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SOLAR-POWERED AEROGEL-BASED ADSORPTIVE AIR CONDITIONING

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SOLAR-POWERED AEROGEL-BASED ADSORPTION-TYPE AIR CONDITIONING

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Abstract

The DOE estimates the total primary energy consumption for commercial buildings was 10.72 quadrillion BTU (quads) in 1983, compared with 14.74 quads for the residential sector. According to the DOE Building Technologies Program, 40–60% of the energy used in U.S. commercial (and residential) buildings is for HVAC, creating massive potential for energy savings with a system that could cut cooling energy use by at least 30–60%. Initial vertical segments in the commercial building market include government and commercial office buildings; government facilities such as prisons, military bases, and schools; hotels and resorts; farming, wineries and other rural facilities; and general light industrial offices (e.g., printers and clothing makers). We propose a solar-powered aerogel-based adsorption cooling system, including the completion and testing of a working prototype at an existing HVAC testing facility and technology-maturation testing at an existing beta-testing site.

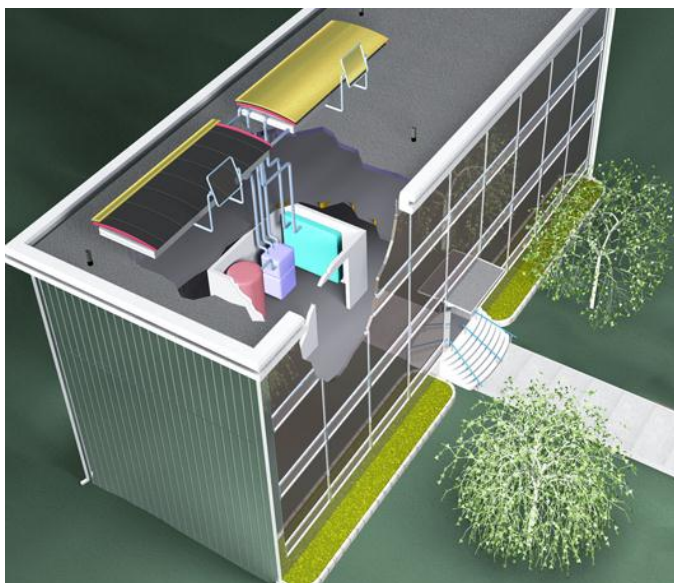


Figure 1 – Solar powered HVAC system with ultra high surface area aerogel adsorption media on the roof of building.

In the cooling system, solar radiation is focused by solar collectors onto on bed, which contains ultra high surface area aerogel. Heating causes thermal desorption of a refrigerant previously adsorbed into the aerogel's pores. Refrigerant desorption increases the gas-phase pressure in the pores, thereby forcing the gaseous refrigerant to flow out of the first irradiated bed (Bed A) and through a two-stage condenser. In the condenser, heat is first removed from the hot gaseous refrigerant by a stream of water that eventually flows into a hot water heater and storage system. The refrigerant is then further cooled by chilled refrigerant leaving the evaporator after vaporization. After passing through the two-stage condenser, the gaseous refrigerant undergoes expansion through an expansion valve. A portion of the refrigerant condenses in the evaporator, while some of the refrigerant is flashed and exits the evaporator. The evaporator absorbs heat from the area being cooled, which results in further vaporization of the refrigerant. The cool, vaporized refrigerant leaves the evaporator, passing through tubes in the shell-and-tube heat exchanger comprising the second stage of the two-stage condenser. After leaving the tube side of this heat exchanger, it flows to the second bed of aerogel (Bed B), which is maintained at a relatively low temperature by water entering the building and destined for the hot water tank. During the first cycle, most of the refrigerant adsorbs on Bed B. When the refrigeration cycle is reversed, the refrigerant is thermally desorbed from Bed B, and adsorbed on the cooler Bed A. As the cycling rate increases, the quantity of adsorption media, the system size, and the associated cost becomes smaller. It appears that an optimized system can meet targeted performance.

List of Acronyms

AC	activated carbon
AMS	Advanced Materials Science [Group] (LLNL)
BET	Brunauer–Emmett–Teller [theory]
CA	carbon aerogel
CFC	chlorofluorocarbon
CMMD	Condensed Matter and Materials Division (LLNL)
CRADA	cooperative research and development agreement
CSD	Chemical Sciences Division (LLNL)
DHS	Department of Homeland Security
EDAX	energy-dispersive analysis of x rays
EER	energy efficiency ratio
ESEM	emission scanning electron microscopy
ETD	Engineering Technologies Division (LLNL)
FTE	full-time employee
HVAC	heating, ventilation, and air conditioning
IPO	Industrial Partnerships Office
LLNL	Lawrence Livermore National Laboratory
NREL	National Renewable Energy Laboratory
PI	principal investigator
SEER	seasonal energy efficiency ratio
T&P	temperature and pressure
TEM	transmission electron microscopy
TFG	Thermal Fluidics Group (LLNL)
UHS	ultrahigh surface (carbon aerogel)

Research and Development Tasks

Overall Purpose

This proposal supports the goal of achieving net-zero-energy building capabilities by 2025, and aims to develop a solar-driven aerogel-based adsorption cooling system. This concept directly converts solar heat to the work of compression necessary to drive the adsorption-based refrigeration system. The outer surface of the pressure envelope surrounding the adsorption bed will be coated to maximize the absorption of solar radiation. This system leverages LLNL's aerogel nanotechnology for dramatic enhancements in the active surface area of the adsorptive media. LLNL can make carbon aerogels and other foam-like materials with surface areas over 3000 m²/g. In contrast, materials currently used in more conventional adsorption cooling systems, which include silica gels, zeolites and activated carbons, have areas of 100-1500 m²/g.

Underlying Hypotheses and Technical Concepts

The underlying hypotheses for the proposed concept are: (1) solar-driven thermal desorption of a refrigerant from a suitable high-surface area media can be used instead of mechanical compressors as the basis of an efficient refrigeration cycle, thereby reducing the need for electrical power from grids for cooling homes and offices; (2) sorption capacity is proportional to specific surface area, with the adsorption of approximately 10¹⁴ molecules per square meter in some cases; (3) the higher surface area attainable with carbon aerogels can reduce the required mass of the adsorption bed, thereby enabling the construction of an adsorption-type air conditioning system of lower weight and smaller size relative to those relying on commercially available sorbent materials; (4) carbon aerogel can be fabricated as monolithic flat sheets for optimal heat and mass transfer in the adsorption bed; (5) carbon aerogels can be readily modified to tune the thermodynamics of adsorption, providing flexibility in the selection of refrigerants—including non-CFCs—and in operating temperatures; (6) injection-molded silica aerogel has the highest heat transfer resistance of any known engineered material and can be used to control heat leakage in the system, thereby increasing overall efficiency; (7) by eliminating moving parts, longer service life, lower maintenance costs and lower levels of noise can be achieved.

Specific Tasks

This project is organized into 13 tasks: (1) initial synthesis of ultrahigh-surface carbon aerogel (UHS-CA), (2) determination of adsorption isotherms; (3) production of UHS-CA; (4) quality assurance and control of UHS-CA production; (5) computational analysis and design of the system; (6) engineering design of a single-bed system and its components; (7) component fabrication, charging of adsorption bed, system assembly, and installation; (8) performance testing and demonstration; (9) calibration and validation of a computational model for system design; (10) design and optimization of two-bed temperature-swing prototype; (11) performance testing and demonstration of the two-bed temperature-swing prototype; (12) high-performance thermal insulation enhancement; and (13) technology transfer and commercialization. Progress in each task will be documented in a quarterly report, with the progress made after four quarters summarized in an annual report. This seedling proposal requests \$500K over two years with a 20% in-kind match by the industrial partner, Ocellus for execution of tasks 1 through 8, the initial demonstration of the concept.

Research and Development Strategy

Innovation

Solar-driven adsorptive cooling systems have been under active development for over two decades. Existing systems range in complexity from very simply constructed single-bed, single-loop designs to multi-stage, multi-bed regenerative systems for industrial applications, but these often use industrial waste heat rather than solar energy. The simpler, single-bed designs have been suggested for residential rooftop and often call for water or ammonia as the refrigerant and activated carbon, silica gels, or zeolites as the adsorbent. Some water-based systems generate ice blocks for thermal mass, while most systems depend on liquid evaporation as the primary cooling mechanism. The closest related technology to the proposed system is absorptive cooling, in which the refrigerant is absorbed and desorbed from the adsorbent through a bulk mixing of the phases. The thermodynamic cycle is similar to adsorptive cooling and can be driven by solar power. Absorptive systems, however, suffer from corrosion and high maintenance costs compared to adsorptive systems. The chiller is a solar-energy-fired absorption unit producing chilled water (3–5°C) to cool the building. Conventional evaporative (i.e., swamp) coolers may be used in dry climates as they rely on low relative humidity to function but have limited effectiveness, cannot produce a significant temperature drop, and require water resources. However, the proposed system is distinguished by aerogel's ultrahigh surface area density and its far greater cooling efficiency.

Aerogels are among the most versatile materials available owing to their wide variety of exceptional properties. For example, aerogels are known to exhibit the lowest thermal conductivities (0.017–0.021 W/m·K), sound velocities (<500 m/s), and refractive indexes (1.001–1.15) of any bulk solid material. Most of the properties of bulk aerogels are also exhibited in other forms of the material, such as thin sheets or films, which is important for integration of these materials into devices. As a result, aerogels have been developed for a variety of applications, including catalysis, sensing, thermal insulation, waste management, molds for molten metals, optics, capacitors, energetic composites, imaging devices, cosmic dust collection, and high-energy-density physics applications. LLNL is recognized as a world leader in aerogel research, holding several patents in the technology dating back to the mid-1990s. Organic and carbon aerogels were both invented at LLNL, and much of the technology resulting from that research has been licensed for various technologies, including capacitors and desalination. The process used to synthesize high-surface-area carbon aerogel adsorbents was also developed at the Laboratory, where the materials are currently used as adsorbents for hydrogen in low-pressure storage tanks. We have the requisite facilities to scale up production of these materials to meet the needs of this effort. In addition, the rapid supercritical extraction (RSCE) process that will be used to fabricate the insulating aerogel parts was developed and patented by LLNL. The RSCE process—very similar to injection molding, a common process used to manufacture some plastics—offers a number of advantages over conventional supercritical drying, including simpler and less costly hardware, monolithic gels that do not have to be pre-formed, and an overall much faster process—the entire process for making monolithic parts can be accomplished in just a few hours instead of the several days required by conventional supercritical drying. The RSCE process will be extremely valuable in the fabrication of conformable monolithic for the proposed cooling system's insulation.

Approach

According to the market assessment group Frost and Sullivan, “Even though renewable energy technologies integrated with HVAC systems are presently holding a negligible share in the U.S. market, they are poised to gain significant momentum over the next decade. This trend is driven by factors such as the demand to reduce carbon emissions, legislation, and expected cost competitiveness. Regulatory bodies, environmental consciousness, price, and efficiency-sensitive customers are positively influencing the technological capabilities and competitive structure of the HVAC equipment markets.” Another market assessment group, Reportlinker, expects U.S. demand for HVAC equipment to increase 4.5% annually through 2013 to \$17 billion, buoyed by an expected rebound from the current sluggish economy. Two market segments exist for commercial HVAC systems: new buildings and retrofitting. Although the retrofit market is very conservative—most building owners do not consider a retrofit until the existing HVAC system is very old or has ceased to function—tax credits and other government

stimulation are providing unprecedented interest and growth in both of these segments. Even if market penetration occurs slowly, even at half a percent per year, we can use the aforementioned market estimate of \$17 billion to forecast almost \$13 million in growth every year. Market strategies that will fortify and increase market penetration are (1) market promotion, e.g., in industry trade journals read by building managers and also by the mass media, given today's heightened interest in Earth-friendly technologies; (2) low-risk offers, i.e., limiting the amount of retrofit that needs to be done by providing units that work seamlessly with existing HVAC systems; and (3) energy audit follow-ups. We assumed that the target market will about 80% of the continental U.S. for space cooling and water heating and about 56% of the continental U.S. for space heating, with the New England, the Mid-Atlantic, and the East North Central regions expected to exhibit a significantly lower likelihood of technology adoption because of lower available average solar fluence.

This proposal, in support of the goal of achieving net-zero-energy building capabilities by 2025, aims to develop a solar-driven aerogel-based adsorption cooling system. This invention directly converts solar heat to the work of compression necessary to drive the adsorption-based refrigeration system. The outer surface of the pressure envelope surrounding the adsorption bed will be coated to maximize the absorption of solar radiation. This system leverages LLNL's aerogel nanotechnology for dramatic enhancements in the active surface area of the adsorptive media. For example, LLNL can make carbon aerogels with surface areas over 3000 m²/g. In contrast, materials currently used in adsorption cooling systems—commercially available silica gels, zeolites, and activated carbons—exhibit much lower surface areas, typically 100–1500 m²/g. Since sorption capacity is proportional to specific surface area, with the adsorption of approximately 10¹⁴ molecules per square meter in some cases, the higher surface area attainable with carbon aerogels can reduce the required mass of the adsorption bed, for an air conditioning

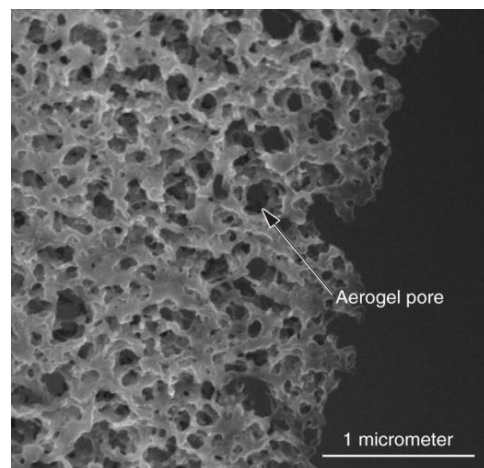


Figure 2 – LLNL's aerogels are some of the highest surface-area materials on Earth. Their extreme porosity allows the material to hold large quantities of refrigerant adsorbed onto its pore surfaces.

system of lower weight and smaller size compared to what is possible with commercially available sorbent materials. Carbon aerogel can be fabricated as monolithic flat sheets for optimal heat and mass transfer in the adsorption bed. (These monolithic sheets of aerogel can be bonded to the inner surfaces of the pressure envelope surrounding the adsorption bed.) This reduces cost and eases installation by eliminating the need for fin-shaped beds. In addition, the carbon aerogels can be readily modified to tune the thermodynamics of adsorption, providing flexibility in the selection of refrigerants—including non-CFCs—and in operating temperatures. To assure exceptional thermal insulation we propose using injection-molded silica aerogel for thermal insulation. This insulation has the highest heat transfer resistance of any known engineered material and will therefore help control heat leakage in the system, increasing overall efficiency. Using the adsorption bed itself for compression, this

- Most compact beds of any adsorption-based cooling scheme.
- No moving parts, for durability and ease of maintenance.
- Enhanced solar collection using optics design suitable for cold climates.
- Thermal modeling to minimize risk.
- HVAC engineering to assure marketability.
- Experience in commercialization and industrial-scale aerogel production.

system will have no moving parts, which assures long service life and low maintenance costs, eliminates the need for lubricants, and dramatically reduces cooling-system noise. The use of a hermetically sealed pressure envelope containing the refrigerant is enabled by the elimination of moving parts and electrical feed-through. This will minimize the probability of refrigerant leakage from the system and eliminate the need for periodic recharging with makeup refrigerant, which will also reduce operating costs and environmental burden. Livermore's optic design expertise, such as Fresnel optics originally developed for space-based applications, can be used to enhance solar concentration and increase the upper operating temperature of the adsorption bed during thermal desorption, thereby achieving higher compression and greater efficiency, making the system suitable for high latitudes, cold climates, and cloudy days. The system will have an integrated hot water heater. The system will also have sufficient flexibility to use fossil fuel or electricity for auxiliary heating and to operate from other heat sources, including waste heat from automotive engines, industrial plants, and nuclear power plants. HVAC system optimization will assure retrofitability, including compatibility with existing ventilation systems.

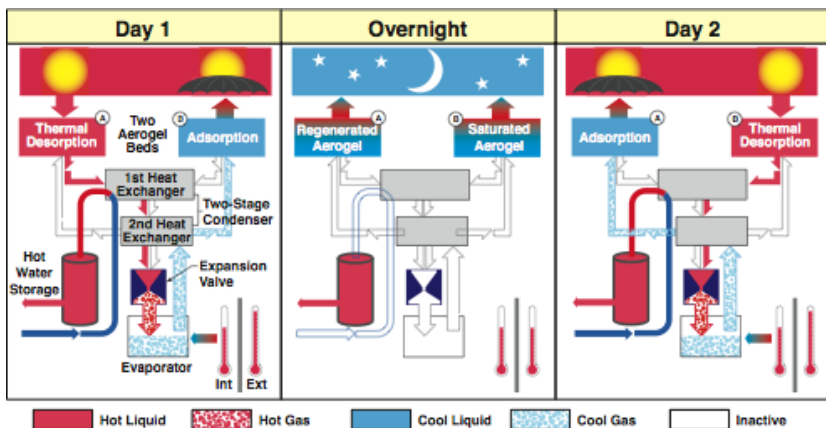


Figure 3 – Schematic of solar-powered adsorptive refrigeration cycle used for building HVAC applications.

SOLAR COLLECTOR – Many conventional solar concentrators rely on parabolic mirrors to heat pipes located at the focal points of the mirrors. In the case of adsorptive refrigeration and cooling systems, this dictates that the adsorption media be placed in a cylindrical envelope for the most efficient heating. Alternatively, large inexpensive Fresnel optics, now available can be used for solar collection from the solar-side of planar panels, providing designers with some engineering advantage. For the solar collectors, this project will bring to bear LLNL's extensive experience in designing optics. We expect to use commercially available molded acrylic lenses or reflective concentrators. We will also leverage Livermore's extensive optics design experience to focus on cost reduction and including space heating options with cooling to promote market penetration.

AEROGEL ADSORPTION-DESORPTION BEDS – Carbon aerogel (CA) is a unique porous solid with network structures consisting of interconnected carbon particles and, as a result, these materials exhibit many interesting properties, such as high surface-to-volume ratios, continuous porosities and high electrical conductivity. Lawrence Livermore National Laboratory has developed a synthetic approach to fabricate CAs with BET surface areas of over 3,000 m²/g. These surface area values are the highest that we are aware of for CAs and are comparable to those of the highest surface area activated carbons. Our synthetic strategy involves the thermal activation of a CA material with structural features (particles and pores) on the micrometer scale. This approach not only provides access to high surface areas in CA materials but also affords monolithic materials with bimodal porosity (macro- and micropores).

An important criterion for effective physisorption is a high surface area that exposes a large number of sorption sites to ad-atom or ad-molecule interaction. Moreover, these sites need to have potential wells that are sufficiently deeper than kT if physisorbents are to operate at reasonable engineering temperatures. Porous carbon materials are promising candidates for the physisorption of refrigerant gases due their lightweight frameworks and high accessible surface areas. High surface area carbons have been studied extensively for low pressure storage of transportation fuels, such as hydrogen and methane. For example, appreciable amounts of methane can be adsorbed on conventional high surface area activated carbons at 298 K and 3.5 MPa. More specifically, the loading of CH₄ on such activated carbons is approximately 17 weight percent or 0.17 grams of methane per gram of solid carbon. Carbon aerogels (CAs) are a unique class of porous carbons that possess ultrafine cell sizes, continuous porosities and low mass densities. These properties arise from the aerogel microstructure, a three-dimensional network of interconnected primary carbon particles with diameters that can range from a few nanometers to several microns. We recently developed a synthetic approach at LLNL to fabricate mechanically robust CA monoliths with BET surface areas in excess of 3,000 m²/g of carbon aerogel, substantially greater than that achievable with the best activated carbons. These surface area values are the highest reported for CAs and exceed the accessible surface area in most commercially available activated carbons. In addition to extremely large specific surface areas,

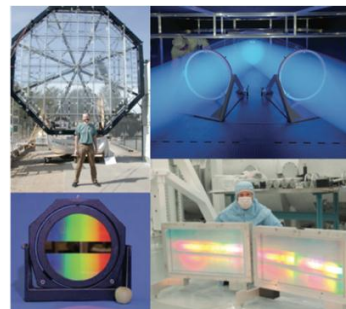


Figure 4 – Ultimately, for enhanced solar collection, Livermore's extensive optics design experience, such as large-format Fresnel optics (upper left) and optics developed for the National Ignition Facility. Improved solar collection will allow the system to be used in colder climates

these materials exhibit a number of other desirable qualities for the adsorption of refrigerant gases. First, the porosity in these CAs is bimodal, consisting of a large population of micropores (0.7 to 1.2 nanometers in diameter) connected by a continuous macroporous network. Hierarchically porous carbons of this type are superior to carbons with unimodal porosity (i.e. activated carbons) in terms of diffusion efficiency and surface area. The surface chemistry of the CA can be readily modified to tune the interaction (binding energy) between the refrigerant gas and the adsorbent. This aspect will be particularly important for controlling desorption of refrigerant from the CA during solar heating. These materials do not require the specialized drying processes (i.e. supercritical extraction) that are typically employed in the synthesis of other aerogel materials, minimizing both the fabrication time and cost associated with these materials. Finally, unlike many other porous carbons, the CAs can be fabricated in a variety of forms, including conformable monoliths, a feature that can be advantageous for this application. The flexibility associated with the design of these materials should allow us to optimize not only adsorbate-adsorbent interactions, but also maximize the gravimetric and volumetric capacities of these CA materials. Therefore, we believe that these high surface area CAs offers viability to engineer an efficient adsorbent bed for refrigerant gases.

CONDENSER OPTIONS – The proposed system may use a two-stage condenser to cool and condense the desorbed refrigerant. The first stage will use an external water stream, resulting in a hot water stream for other uses. The second stage will be chilled by the return line of evaporated and expanded refrigerant.

EVAPORATOR OPTIONS – The evaporator is a two-phase boiler with both liquid and gaseous refrigerant. Liquid is continuously evaporated as heat is absorbed from the building primary heat exchanger. The primary heat exchanger can be of any conventional design, which will allow easy retrofit of the proposed system into new or existing construction.

HIGH-PERFORMANCE AEROGEL THERMAL INSULATORS – Silica aerogels are a special class of open-cell foams derived from highly cross-linked gels that are dried using special techniques (supercritical extraction) to preserve the tenuous solid network. These materials have ultrafine cell and pore sizes ($<1,000 \text{ \AA}$), continuous porosity, high surface area density, and a microstructure composed of interconnected colloidal-like particles or polymeric chains with characteristic diameters of 100 \AA . This microstructure is responsible for the unusual optical, acoustical, thermal, and mechanical properties of silica aerogels. In fact, silica aerogels have the lowest thermal conductivity ($0.017\text{--}0.021 \text{ W/m}\cdot\text{K}$) of any solid material and, as a result, have been commercially developed for thermal insulation applications. These materials are ideal insulators for the proposed AC system. The rapid supercritical extraction process used to fabricate these materials is scalable and can be used for high-throughput production of insulating parts.

AIR HANDLING, SENSORS AND CONTROL SYSTEM – These components will be designed to be compatible with existing building ventilation systems.

Detailed Description of Tasks for Proposed Effort

We will design, build, install, and test an aerogel-based solar-powered adsorptive air conditioning system for low-rise commercial buildings. The system will directly convert solar heat to the work of compression necessary to drive the system. The adsorption–desorption bed material will consist of an advanced nananostructural aerogel whose high surface area density permits much smaller beds than would activated carbon-based sorption materials. The system will there be compact and, having no moving parts, easy to maintain and easy to retrofit into existing buildings. High thermal efficiency and enhanced solar collection will permit operation in cold climates.

PROJECT TASKS – This project is organized into 13 tasks, with the first 9 tasks done during this seedling project, and the last 4 tasks done during future work aimed at commercialization: (1) initial synthesis of ultrahigh-surface carbon aerogel (UHS-CA), (2) determination of adsorption isotherms; (3) production of UHS-CA; (4) quality assurance and control of UHS-CA production; (5) computational analysis and design of the system; (6) engineering design of a single-bed system and its components; (7) component fabrication, charging of adsorption bed, system assembly, and installation; (8) performance testing and demonstration; (9) calibration and validation of a computational model for system design; (10) design and optimization of two-bed temperature-swing prototype; (11) performance testing and demonstration of the two-bed temperature-swing prototype; (12) high-performance thermal insulation enhancement; and (13) technology transfer and commercialization. Progress in each task will be documented in a quarterly report, with the progress made after four quarters summarized in an annual report.

Seedling Project

TASK 1 – INITIAL SYNTHESIS OF ULTRA HIGH SURFACE CARBON AEROGEL: Once funds are available, procurements of those materials and chemicals necessary for the synthesis of the required aerogels will be made. It is estimated that adsorption isotherm studies will require approximately 5 kg of UHS-CA, while the single-bed prototype will require approximately 613 kg of UHS CA, and approximately 159 kg of refrigerant (these estimates are subject to revision as better data becomes available). While much of the UHS CA synthesized for the single-bed prototype can be re-used in the two-bed temperature swing prototype, some additional aerogel may be required to compensate for adsorption media unavoidably damaged during system reconfiguration. We will prepare a series of high surface area CAs to screen as adsorbents for select refrigerant gases. The CAs are prepared through the sol-gel polymerization of resorcinol and formaldehyde in aqueous solution to produce highly cross-linked organic gels that are dried under ambient conditions and subsequently pyrolyzed in an inert atmosphere. To increase the accessible surface area in these materials, the CAs are then thermally activated with carbon dioxide. To optimize the performance of the CA adsorbents, we will investigate the influence of micropore size on the uptake and storage of the refrigerant gas. Previous studies have shown that size and shape of the pores in physisorbents play a critical role in uptake of adsorbate gases. For example, the optimal pore structure for the adsorption of methane on carbon are slit-shaped pores with diameters of ~1.1 nm. For the work proposed here, the average size of micropores in our sorbents can be tuned through modifications in the activation process. In addition, we will also evaluate the impact of CA surface chemistry (i.e. oxygen-containing groups) on the binding

energies for the different refrigerant gases. The surface characteristics of these CAs can be readily modified using vapor phase techniques without compromising the high specific surface areas of the adsorbents. For example, these CA can be coated with a thin layer of silicon dioxide to produce a new UHS material with adsorption characteristics similar to those of silica gel. This ability to modify both porosity and surface chemistry in the CA sorbents provides significant latitude in the selection of the refrigerant gas. The influence of these factors on adsorption will be evaluated in Task 2 of this effort. In later phases of this effort, we will also investigate alternative UHS adsorbent materials, such as metal-organic frameworks (MOFs). MOFs are crystalline compounds consisting of metal ions (or clusters) coordinated to organic spacer molecules to form highly ordered three-dimensional porous structures. The pore structure and surface area of MOFs can be modified through the selection of the organic spacer and metal species, allowing for the fabrication of MOF materials with surface areas as high as 5000 m²/g. Like the CAs, MOFs should provide improved gravimetric capacities of refrigerant gases in the adsorbent bed compared to those reported for conventional adsorbents. MOF materials may also provide the opportunity to tune the thermodynamics of adsorption through selection of the organic spacer and metal species.

TASK 2 – DETERMINATION OF ADSORPTION ISOTHERMS: The performance of the CA adsorbents will be evaluated by measuring the adsorption isotherms of the refrigerant gases on the various adsorbents. The investigative team will select the most promising candidates for testing as adsorbents in prototype systems. An experimental measurement apparatus will be constructed to determine the surface coverage of UHS-CA by both halogenated and non-halogenated candidate refrigerants as a function of temperature and pressure. This experimental apparatus will be relatively simple, and will involve two small temperature-controlled vessels, one containing approximately 5 kg of adsorption media (UHS-CA), and the second containing a sufficient quantity of refrigerant exceed the saturation coverage of the UHS-CA over the entire range of temperature to be investigated (–40 to 200°F). The two stainless steel vessels will be connected via low-weight flexible tubing and a precision control valve. Each of the vessels will have independent pressure transducers, and will be suspended from piezoelectric load cells to enable precise determination of the weights of the vessels and contents. The pressure transducer and load cell on the refrigerant vessel will provide redundant measurements of refrigerant inventory in the vessel. Once the precision control valve leading to the vessel with UHS-CA is opened, refrigerant will move into the UHS-CA vessel and begin adsorbing on the surface of the material. The total mass flow into from the refrigerant vessel into the UHS-CA vessel can be determined from the pressure transducer and load cell data from the refrigerant vessel. The partitioning of refrigerant between the gas and adsorbed phases in the UHS-CA vessel can be determined from the pressure transducer and load cell data from the UHS-CA vessel. This methodology will then be incorporated into the single-bed prototype, to enable precise monitoring of performance. By varying the pressure and temperature in the vessels, the adsorption isotherms for conventional halogenated refrigerants on both conventional AC (control data) and the UHS-CA can be determined. These measurements will be repeated for non-halogenated refrigerants, thereby determining the adsorption isotherms for refrigerants such as normal and isobutene, propoane, and ammonia on the UHS-CA. The work can be extended to investigate other potential refrigerants with UHS-CA such as carbon dioxide. The results of this task will also be used to refine the synthesis of the carbon aerogel adsorbents as part of Task 1.

TASK 3 – PRODUCTION OF UHS-CA: Once reliable data are available from the adsorption isotherm studies, it will be possible to estimate the amount of UHS-CA needed for construction of a single-bed prototype cooling system. At that point, synthesis will commence so that a sufficiently large enough quantity of UHS-CA can be produced to fill single adsorption bed for working prototype. Additional chemicals may have to be procured. Initial estimates indicate that a minimum of 613 kg of UHS-CA will be required for this activity, with an estimated cost for reagent grade chemicals of approximately \$12,000 (cost for commercial production will be substantially less).

TASK 4 – QUALITY ASSURANCE & QUALITY CONTROL OF UHS-CA PRODUCTION: The morphology, microstructure and elemental purity of the UHS-CA produced during execution of Task 3 will be determined with pre-existing environmental scanning electron and transmission electron microscopes (ESEM & TEM). Both have the ability to perform measurements of elemental composition with attachments that enable energy-dispersive analysis of x-rays (EDAX). The density will be determined from measurements of weight and volume using calibrated digital balances. The effective surface area of the HUS-CA will be determined with BET surface analysis using nitrogen gas. As a final quality assurance–control measurement, the Langmuir parameters (saturation loading, free energy of adsorption, and pre-exponential) will be determined for the two leading refrigerant candidates. Data will be compared to original isotherm data as a means of qualifying the production-run material. If for any reason the material does not have the anticipated properties, a root cause analysis will be performed and the production process will be repeated with necessary corrections.

TASK 5 – COMPUTATIONAL ANALYSIS & DESIGN OF SYSTEM: A computational model, and then use that model for the engineering design of a single-bed prototype with controllable heater, adsorption bed, condenser, expansion valve, evaporator, ballast volume, sensors and control system. The system design process will begin with a fundamental thermodynamic analysis of the system, considering the external heat exchange boundaries, enthalpy cycle of the refrigerant, and the irrecoverable losses (2nd law analysis). Numerical system behavior models will be developed that capture the transient response of the entire system under various operating scenarios to develop a performance database. These models may be evaluated over seasonal variations to predict EER and SEER performance. Detailed thermal-fluid-mechanical studies of individual components, such as the adsorptive beds, will be performed for physical understanding and optimization. Predicted performance will be validated against prototype testing at both component and system scales.

TASK 6 – ENGINEERING DESIGN OF SINGLE-BED SYSTEM AND COMPONENTS : The abstract process model will be translated into the practical design of system components by Mr. that can be procured, or fabricated in the machine shops at Livermore, or the surrounding area by Livermore's lead HVAC engineer, Mr. Robert Simonds, with the assistance of Drs. Wayne Miller and Joseph Farmer, with advice from Drs. Ted Baumann and Joseph Satcher. Triple-A engineering drawings will be generated for each of the major components that has to be fabricated for construction of the a working prototype with a single adsorption bed. These drawings will undergo a formal design review by other mechanical engineers at Livermore, and following approval, will be provided to the machine shop so that components can be fabricated.

TASK 7 – COMPONENT FABRICATION, ADSORPTION BED CHARGING, SYSTEM ASSEMBLY AND INSTALLATION: Components that will be procured or fabricated include: a controllable heater; adsorption bed; condenser and other necessary heat exchangers; expansion valve; evaporator, ballast volume, sensors and control system. Any components for single-bed prototype that cannot be procured will be fabricated in accordance with the formal engineering drawings generated during execution of Task 6. Following fabrication of all components, and preceding assembly into a system, the containment volume for the adsorption bed will be charged with ultra high surface CA. Then, procured and fabricated components, and any pre-existing components, will be assembled into a functional prototype for installation and testing. In parallel with the procurement, fabrication and assembly process, all necessary work permits for installation and testing of the prototype on Livermore's pre-existing HVAC laboratory will be obtained. Following assembly, and with all necessary approvals, the system will be installed on Livermore's pre-existing HVAC laboratory for the initial performance testing.

TASK 8 – PERFORMANCE TESTING AND DEMONSTRATION: The assembled and installed single-bed prototype will be fully instrumented, and used to perform screening studies, to verify selection of the best combination of ultra high surfaced area CA and refrigerant. The instrumented single-bed cooling unit, charged with the best combination of ultra high surface area CA and refrigerant will then be used to demonstrate the systems performance capabilities, using a controllable surrogate electrical heater to drive the system. Once operation is demonstrated with the controllable electrical heater, the surrogate electrical heating unit will be replaced with a solar collection system, thereby enabling demonstration of the system with solar heating. The initial demonstration will be scheduled for peak solar in middle of the California summer, with additional demonstrations during other seasons, using the summer demonstration as a standard for comparison. The apparent SEER, EER and COP of the single-bed prototype will be determined, reviewed by a peer review panel, and then published.

TASK 9 – CALIBRATED & VALIDATED COMPUTATIONAL MODEL FOR SYSTEM DESIGN: The credible development of a cooling unit for commercialization and wide-spread use will require further development of the computational model, thereby enabling detailed thermal analysis of the transient cooling system. Once calibrated and validated, this computational design tool can be used for optimization of the hardware and control system. Data obtained during the initial performance testing of the single-bed prototype will be used for the calibration of model parameters. Additional experiments for model validation.

Future Work Required for Commercialization

TASK 10 – DESIGN AND OPTIMIZATION OF TWO-BED TEMPERATURE-SWING PROTOTYPE: The credible development of a cooling unit for commercialization and wide-spread use will require further development of the computational model, thereby enabling detailed thermal analysis of the transient cooling system. Once calibrated and validated, this computational design tool can be used for optimization of the hardware and control system. Data obtained during the initial performance testing of the single-bed prototype will be used for the calibration of model parameters. The calibrated and validated computational model will be used to design a continuous two-bed prototype, with an emphasis on using temperature swing refrigerant adsorption as a means of decreasing the inventory of adsorption media and

refrigerant, thereby lowering overall cost. A continuous two-bed prototype will be designed and optimized, using the model. To the extent possible, the two-bed prototype will be constructed through modification of the initial single-bed prototype, thereby enabling operation with two parallel beds at a phase-angle difference of 180 degrees, each half the size of the original single bed. Designs with more than two-beds, and more complex phasing will also be considered as a means of achieving performance enhancements.

TASK 11 – PERFORMANCE TESTING AND DEMONSTRATION OF TWO-BED TEMPERATURE-SWING PROTOTYPE: The initial performance testing of the two-bed temperature-swing prototype will be conducted with two calibrated electrically-powered surrogate heaters. To the extent possible, a demonstration will be conducted, showing that such a temperature-swing system has a higher mass-specific refrigeration capacity than possible with single-bed operation, and is therefore smaller and more cost effective. Following demonstration with two surrogate electrical heaters, the system will undergo slight modification, thereby enabling demonstration of the temperature-swing adsorption system with solar collectors capable of phased heating of the two parallel adsorption beds. The apparent SEER, EER and COP of the two-bed temperature prototype will be determined, reviewed by a peer review panel, and then published.

TASK 12 – HIGH-PERFORMANCE THERMAL INSULATION ENHANCEMENT: Once the two-bed temperature-swing prototype is demonstrated, silica aerogels, known to have the lowest thermal conductivity of any known engineering material will be integrated into the system as thermal insulation. This will result in substantial performance enhancement of the system, and further leverage DOE's long-standing investment in this specific nano-technology.

TASK 13 – TECHNOLOGY TRANSFER AND COMMERCIALIZATION: Prior to widespread dissemination of proprietary data, all conceptual and actual designs, and performance data will be reviewed, using formal records of invention, provisional patents, domestic and foreign patent filings, and declaration of trade secrets for fortification of intellectual property (IP) portfolio. This will be essential for successful commercialization, since any such device without appropriate IP protection will be difficult to transition. Collaborators will be integrated into the project early, from representatives of the stakeholder community: prospective licensees, prospective commercial users of the technology, and prospective installer/ maintenance workforce development candidates. To streamline technology development, the commercialization plan includes integration of these stakeholders into technology development activities during the installation of prototype units on buildings, one in the hot, dry summer and cool winter environment found in the Livermore valley, and the other in the hot rainy tropical environment found on the east side of Hawaii.

SUMMARY OF PROJECT DELIVERABLES

Seedling Project

Deliverable 1.1: Procurement of Materials and Chemicals

Deliverable 1.2: Synthesis of 1st 5-kg Batch of UHS-CA with BET Surface Area $> 3000 \text{ m}^2/\text{g}$

Deliverable 2.1: Design & Construction of Apparatus for Isotherm Determination

Deliverable 2.2a: Adsorption Isotherms for Halogenated Refrigerants & conventional AC

Deliverable 2.2b: Adsorption Isotherms for Halogenated Refrigerants & UHS-CA

Deliverable 2.2c: Adsorption Isotherms for Non-Halogenated Refrigerants & conventional AC

Deliverable 2.2d: Adsorption Isotherms for Halogenated Refrigerants & UHS-CA

Deliverable 3.1: Procurement of Additional Materials and Chemicals

Deliverable 3.2: Synthesis of 2nd 100-kg Batch of UHS-CA with BET Surface Area $> 3000 \text{ m}^2/\text{g}$

Deliverable 4.1: ESEM, EDAX & TEM of Samples from 1st 5-kg Batch of UHS-CA

Deliverable 4.2: Determination of Density and BET Surface area for 1st 5-kg Batch of UHS-CA

Deliverable 4.3: ESEM, EDAX & TEM of Samples from 2nd 100-kg Batch of UHS-CA

Deliverable 4.4: Density and BET Surface area for 2nd 100-kg Batch of UHS-CA

Deliverable 4.5: Adsorption Isotherms for Refrigerant A on 2nd 100-kg Batch of UHS-CA

Deliverable 4.6: Adsorption Isotherms for Refrigerant B on 2nd 100-kg Batch of UHS-CA

Deliverable 5.1: Conceptual Design of Single-Bed Prototype

Deliverable 5.2: Preliminary Spreadsheet Model of Single-Bed System

Deliverable 5.3: Comprehensive Computational Model for Transient Operation

Deliverable 5.4: Initial Calibration of Model Parameters with Adsorption Isotherm Data

Deliverable 5.5: Thermal Analysis of Single-Bed Prototype

Deliverable 6.1: Engineering Drawings for Construction of Single-Bed Prototype

Deliverable 6.2: Engineering Drawings of Components for Single-Bed Prototype

Deliverable 6.3: Procure Commercially Available Components for Single-Bed Prototype

Deliverable 7.1: Fabricated Components for Single-Bed Prototype

Deliverable 7.2: Procured Components for Single-Bed Prototype

Deliverable 7.3: Charging of Adsorption Bed for Single-Bed Prototype Assembly

Deliverable 7.4: Fully Assembled of Single-Bed Prototype

Deliverable 7.5: Installation of Assembled Single-Bed Prototype on HVAC Laboratory

Deliverable 8.1: Successful Performance Test of Single-Bed Prototype with Electrical Heater

Deliverable 8.2: Successful Performance Test of Single-Bed Prototype with Solar Heating

Deliverable 8.3: Report Documenting Data from Performance Testing of Single-Bed Prototype

Deliverable 9.1: Successful Performance Test of Single-Bed Prototype with Electrical Heater

Deliverable 9.2: Calibration of Model Parameters with Data from Single-Bed Prototype Testing

Deliverable 9.3: Independent Experiment for Model Validation

Future Work Required for Commercialization

- Deliverable 10.1: Conceptual Design of Two-Bed Temperature-Swing System
- Deliverable 10.2: Reconfiguration of Computational Model for Simulation of Two-Bed System
- Deliverable 10.3: Optimization of Two-Bed Temperature-Swing System
- Deliverable 10.4: Engineering Drawings for Two-Bed Temperature-Swing System
- Deliverable 10.5: Physical Reconfiguration of System as Two-Bed Temperature Swing System

- Deliverable 11.1: Testing of Two-Bed Temperature-Swing Prototype with Electrical Heaters
- Deliverable 11.2: Testing of Two-Bed Temperature-Swing Prototype with Solar Heating
- Deliverable 11.3: Report on Testing of Two-Bed Temperature-Swing Prototype

- Deliverable 12.1: Synthesis of Silica Aerogel for Enhanced Thermal Insulation
- Deliverable 12.2: Retrofit of Two-Bed Temperature-Swing Prototype with Aerogel Insulation
- Deliverable 12.3: Performance Test of System with Enhanced Insulation

- Deliverable 13.1: Comprehensive Records of Invention for Single- and Multi-Bed Systems
- Deliverable 13.2: Comprehensive Patent Applications for Single- and Multi-Bed Systems
- Deliverable 13.3: Copyrights for Pertinent Branding and Trademarks
- Deliverable 13.4: Formal Agreements for Non-LLNL Site Demonstrations
- Deliverable 13.5: One Successful Non-LLNL Site Demonstration
- Deliverable 13.6: Industry Days at LLNL in Collaboration with DOE EERE Program Manager
- Deliverable 13.7: Commercial Licenses for Aerogel-Based Cooling Systems

Preliminary Results

ULTRA HIGH SURFACE CARBON AEROGELS – As described by Livermore's Baumann, Worsley, Han, and Satcher, the design of new porous carbon materials holds technological promise for a variety of applications, including catalysis, adsorption and energy storage [*Journal of Non-Crystalline Solids* 354 (2008) 3513–3515]. The utility of these materials is derived from their high surface areas, electrically conductive frameworks and chemical stability. One area of carbon research that has received significant attention is the use of these porous materials as sorbents for hydrogen. Safe and efficient storage of hydrogen is considered one of the main challenges associated with utilization of this fuel source in the transportation sector. We recently reported on the hydrogen sorption properties of high surface area carbons that were prepared from carbon aerogels (CAs). Carbon aerogels are unique porous solids with network structures consisting of interconnected carbon particles and, as a result, these materials exhibit many interesting properties, such as high surface-to-volume ratios, continuous porosities and high electrical conductivity. In the course of that work, we developed a synthetic approach to fabricate CAs with BET surface areas over 3,000 m²/g. These surface area values are the highest that we are aware of for CAs and are comparable to those of the highest surface area activated carbons. In the work presented here, we describe our approach to the design of these high surface area carbons. Our synthetic strategy involves the thermal activation of a CA material with structural features (particles and pores) on the micrometer scale. This approach not only provides access to high surface areas in CA materials, but also affords monolithic materials with bimodal porosity (macro- and micropores). Hierarchically porous carbons of this type present a number of advantages over unimodal carbon structures in terms of diffusion efficiency and surface area, and thus these materials should also have utility as new catalyst supports or electrodes for electrochemical devices. Thermal activation of CAs involves the controlled burn-off of carbon from the network structure in an oxidizing atmosphere, such as carbon dioxide, resulting in the creation of new micropores as well as opening of closed porosity in the CA framework. Therefore, access to high surface areas in activated CAs requires careful design of the pre-activated carbon framework, as the morphology of the particles that comprise the network structure will ultimately determine the textural properties of the activated material. The microstructure of traditional CAs, consisting of nanometer-sized carbon particles and tortuous pore structures, can both limit the surface areas attainable through activation and lead to inhomogeneous burn-off in monolithic samples. By utilizing CAs with larger pore and particle sizes, however, these issues can be mitigated and monolithic carbons with high surface areas and bimodal pore structures can be readily attained. The synthesis of pre-activated CA structures with larger features can be performed in a number of ways. Carbon aerogels are typically prepared through the sol-gel polymerization of resorcinol with formaldehyde in aqueous solution to produce organic gels that are then supercritically dried and subsequently pyrolyzed in an inert atmosphere. The amount and type of catalyst used in the polymerization reaction dictates the size, shape and connectivity of the primary network particles and, therefore, can be used to influence the structural properties of the resultant CA. One method to generate CAs with larger structural features is the use of low catalyst concentrations in the polymerization reaction. Alternatively, the use of acid catalysts in the sol-gel reaction has also been shown to generate porous structures with network and pore features on the micrometer scale. For the preparation of the CAs used in this study, acetic acid was selected as the reaction

catalyst since the process not only affords macroporous carbon structures, but the monolithic products exhibit enhanced mechanical integrity relative to traditional CAs.

For the synthesis of the pre-activated CA, resorcinol (12.3 g, 0.112 mol) and 37% formaldehyde solution (17.9 g, 0.224 mol) were dissolved in water (15 ml), followed by the addition of glacial acetic acid (0.44 g, 0.007 mol). The reaction mixture was then transferred to glass molds and cured at 80°C for 72 hours. The resultant organic hydrogels were washed with acetone to remove the water and then dried with supercritical CO₂. The organic aerogels were subsequently carbonized at 1050°C for 3 hours under an N₂ atmosphere, yielding CA monoliths with densities 0.55 g/cm³. The activation of these materials was carried out under flowing CO₂ (10 sccm) at 950°C. The activated CAs are designated as ACA-x, where x is the activation time in hours.

Microstructural characterization was performed using scanning electron microscopy (JEOL7401-F). Textural properties were determined using N₂ adsorption–desorption techniques (ASAP 2010 Surface Area Analyzer, Micromeritics). Surface areas and pore volumes were determined using Brunauer–Emmett–Teller (BET) and Barrett–Joyner–Halenda (BJH) methods, respectively, while micropore volumes were calculated from t-plot analysis.

The morphology of the pre-activated CA was evaluated using scanning electron microscopy (SEM). As shown in Figure 5a, the skeletal structure of the pre-activated CA consists of interconnected micron-sized carbon ligaments that define a continuous macroporous network. These ligaments appear to be made up of spherical primary particles that have fused together during network formation. This structural motif is similar to those in previous reports that used acetic acid as the reaction catalyst and is likely responsible for the enhanced mechanical integrity of these CA monoliths. Despite being macroporous, the pre-activated CA still exhibits appreciable surface area (approximately 400 m²/g) due to microporosity within the carbon ligaments.

To determine the effect of activation on the textural properties of this CA structure, cylindrical monoliths of the material were exposed to a stream of CO₂ at 950°C for different soak times. Examination of the activated structures by SEM showed smaller network ligaments relative to the unactivated material (Figure 5b). Each of the activated samples exhibited typical nitrogen adsorption isotherm (Figure 5c). As the activation time is increased, the isotherms for the ACAs show increased adsorption at low relative pressures, indicating the formation of new porosity within the CA monoliths. At shorter activation times, this new porosity is in the form of micropores, as evidenced by the increased micropore volume measured for ACA-2 and ACA-3. At longer activation times, however, these micropores are widened to sizes that cross the micropore/mesopore boundary. The development of super micropores and/or small mesopores is confirmed not only by the diminished micropore volume at longer treatment times but also the slight hysteresis in the isotherm for ACA-6. Nevertheless, the BET surface areas and total pore volumes of the activated materials continue to increase with increasing activation times. While this general trend is similar to those observed in other activated CA systems, the key difference here is that the micrometer-sized network morphology of the pre-activated CA allows access to surface areas in the ACAs in excess of 3000 m²/g. Interestingly, all of the activated materials remained monolithic despite the significant mass loss during thermal treatment.

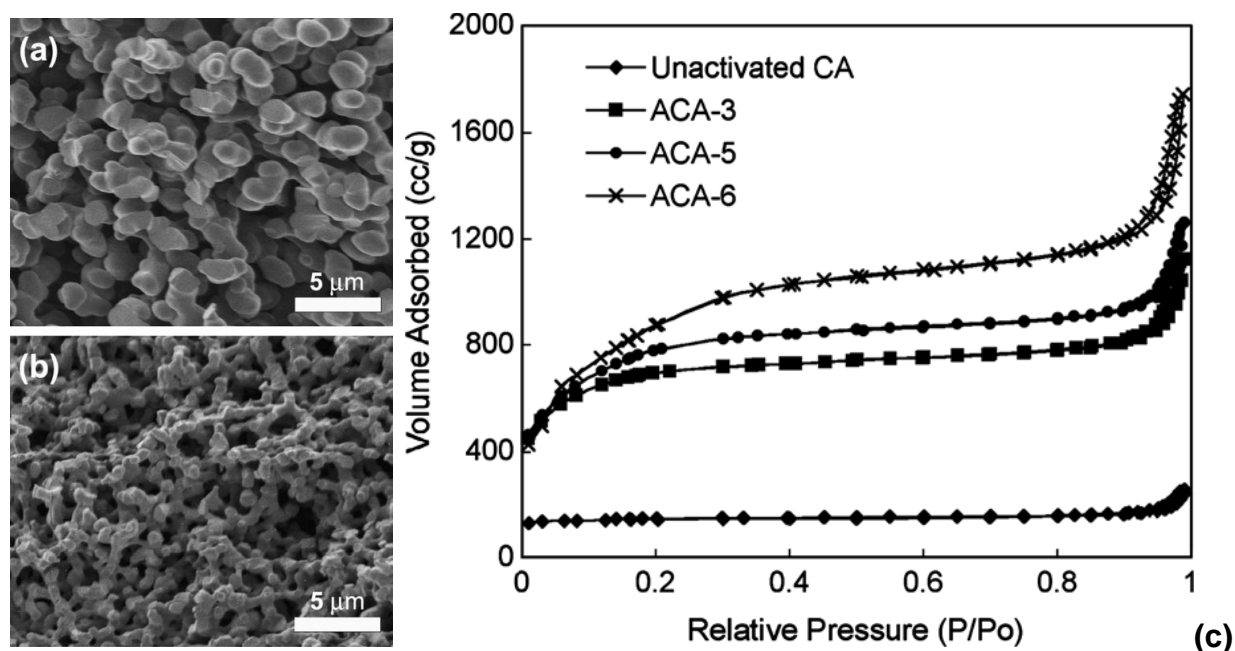


Figure 5 – (a) SEM of pre-activated CA, (b) SEM of activated CA, ACA-6, and (c) BET surface area determination for ACA-3, ACA-5, and ACA-6.

REFRIGERANTS – This proposed system is capable of using a wide variety of environmentally benign non-halogenated refrigerants. Non-halogenated compounds with boiling points appropriate for use as refrigerants are tabulated in Table F1. Similarly, halogenated compounds with boiling points appropriate for use as refrigerants are tabulated in Table F2. We will begin our study assuming the use of iso-butane refrigerant, for which a temperature-dependent Langmuir parameter was estimated with an assumed free energy of adsorption of approximately 45,000 Joules per mole.

Table 1 – Non-halogenated compounds with boiling points appropriate for use in adsorption-desorption refrigeration system.

Name	Formula	FW	BP (°C)	MP (°C)	Density (g/cc)
carbon dioxide	CO ₂	44.0000	-78.6000	-56.6000	1.0310
methyl silane	CH ₃ SiH ₃	46.1200	-57.0000	-156.5000	
propene or propylene	CH ₃ CHCH ₂	42.0800	-47.4000	-185.2000	0.5193
propane	CH ₃ CH ₂ CH ₃	44.1100	-42.1000	-189.7000	0.5831
propadiene or allene	CH ₂ CCH ₂	40.0700	-34.5000	-136.0000	0.7870
ammonia	NH ₃	17.0300	-33.3500	-77.7000	0.7710
cyclopropane	C ₃ H ₆	42.0800	-32.7000	-127.6000	0.7200
dimethyl ether	CH ₃ OCH ₃	46.0700	-25.0000	-138.5000	
methyl acetylene or propyne	CH ₃ CCH	40.0700	-23.2000	-105.5000	0.7062
methyl phosphine	CH ₃ PH ₃	48.0600	-14.0000		
vinyl chloride or chloroethylene	CH ₂ CHCl	62.0500	-13.4000	-153.8000	0.9106
bromo difluoro nitroso methane	BrF ₂ CNO	159.9200	-12.0000		
methyl nitrate	CH ₃ ONO	61.0400	-12.0000	-16.0000	0.9910
isobutane	(CH ₃) ₂ CHCH ₃	58.1200	-11.7000	-159.4000	0.5490
isobutylene	(CH ₃) ₂ CCH ₂	56.1100	-6.9000	-140.3000	0.5942
1-butene	CH ₃ CH ₂ CHCH ₃	56.1200	-6.3000	-185.3000	0.5951
amino methane	CH ₃ NH ₂	31.0600	-6.3000	-93.5000	0.6628
1,3 butadiene or bivinyl	CH ₂ C=CHCH ₂	54.0900	-4.4000	-108.9000	0.6211
butane	C ₄ H ₁₀	58.1200	-0.5000	-138.4000	0.6012
trans 2-butene	CH ₃ CH=CHCH ₃	56.1200	0.9000	-105.5000	0.6042
trimethyl amine	(CH ₃) ₃ N	59.1100	2.9000	-117.2000	0.6356
cis 2-butene	CH ₃ CH=CHCH ₃	56.1200	3.7000	-138.9000	0.6213
1-butene-3-one	CH ₂ CH=CCCH ₃	52.0800	5.1000		0.7095
vinyl acetylene	CH ₂ CH=CCCH ₃	52.0800	5.1000		0.7095
methane thiol	CH ₃ SH	48.1100	6.2000	-123.0000	0.8665
fulvene	C ₆ H ₆	78.1100	7.0000		
1-butyne	CH ₃ CH ₂ CCH ₃	54.0900	8.1000	-125.7000	0.6784
neopentane	(CH ₃) ₄ C	72.1500	9.5000	-16.5000	0.6135
butadiyne	CH ₃ CCCH	50.0600	10.3000	-36.4000	0.7634
1,2 butadiene or methylallene	CH ₂ C=CHCH ₃	54.0900	10.8000	-136.2000	0.6760
cyclobutane	C ₄ H ₈	56.1200	12.0000	-50.0000	1.0457
acetaldehyde	CH ₃ CHO	44.0500	20.8000	-121.0000	0.7834
methanol	CH ₃ OH	32.0400	65.0000	-93.9000	0.7914
cycloheptane	C ₇ H ₁₄	98.1900	118.5000	-12.0000	0.8098

Table 2 – Halogenated compounds with boiling points appropriate for use in adsorption-desorption refrigeration system.

Name	Formula	FW	BP (°C)	MP (°C)	Density (g/cc)
chloro trifluoro methane or Freon 13	ClCF ₃	104.4600	-81.1000	-181.0000	
trifluoro acetonitrile	F ₃ CCN	95.0300	-64.0000		
methylene fluoroide	CHF ₂	52.0200	-51.6000		0.9090
3,3,3-trifluoropropyne	F ₃ CCCH	94.0400	-48.3000		
1,1,1 trifluoroethane	CH ₃ CF ₃	84.0400	-47.3000	-111.3000	
nitroso-pentafluoro ethane	CF ₃ CF ₂ NO	149.0200	-42.0000		
chloroo difluoro methane or Freon 22	ClCHF ₃	86.4700	-40.8000	-146.0000	
chloro pentafluoro ethane	ClCF ₂ CF ₃	154.4700	-38.0000	-106.0000	
fluoroethane	CH ₃ CH ₂ F	48.0600	-37.7000	-143.2000	0.7182
perfluorodimethyl amine	(CH ₃) ₂ NF	171.0200	-37.0000		
perfluoropropane	C ₃ F ₈	188.0200	-36.0000	-183.0000	
perfluoro ethyl amine	CF ₃ CF ₂ NF ₂	171.0102	-35.0000		
trifluoro methyl peroxide	CF ₃ OOCF ₃	170.0100	-32.0000		
nitro trifluoro methane	F ₃ CNO ₂	115.0100	-31.1000		
dichloro difluoro methane or Freon 12	Cl ₂ CF ₂	120.9100	-29.8000	-158.0000	1.1834
perfluoro propylene	CF ₃ CFCF ₂	150.0200	-29.4000	-156.2000	1.5830
1,1,1,2 tetrafluoro ethane	CH ₃ FCF ₃	102.0300	-26.5000		
trifluoro methyl phosphine	F ₃ COH ₂	102.0000	-26.5000		
1,1 difluoro ethane	CH ₃ CHF ₂	66.0500	-24.7000	-117.0000	0.9500
perfluoro 2-butyne	CF ₃ CCCCF ₃	162.0400	-24.6000	-117.4000	
methyl chloride	CH ₃ Cl	50.4900	-24.2000	-97.1000	0.9159
fluoro formaldehyde	FCHO	48.0000	-24.0000		
iodo trifluoro methane	CF ₃ I	195.9100	-22.5000		2.3608
trifluoromethyl sulfide	(CF ₃) ₂ S	170.0800	-22.2000		
trifluoro methane sulfonyl fluoride	F ₃ CSO ₂ F	152.0700	-21.7000		
pentafluoro thio trifluoro methane	F ₃ C(SF ₅)	196.0600	-20.0000		
vinyl chloride or chloroethylene	CH ₂ CHCl	62.0500	-13.4000	-153.8000	0.9106
bromo difluoro nitroso methane	BrF ₂ CNO	159.9200	-12.0000		
1-nitroso heptafluoro propane	CF ₃ CF ₂ CF ₂ NO ₂	199.0300	-12.0000	-150.0000	
trifluoro ethoxyt silane	C ₂ H ₅ OSiF ₃	130.1500	-7.0000	-122.0000	
hexafluorodimethylamine	(CF ₃) ₂ NH	153.0300	-6.7000	-130.0000	
ethyl trifluoro silane	C ₂ H ₅ SiF ₃	114.1400	-4.4000	-105.0000	1.2270
perfluoro cyclobutane	C ₄ F ₈	200.0300	-4.0000	-38.7000	
3-fluoro propylene	FCH ₂ CHCH ₂	60.0700	-3.0000		
perfluoro methyl mercaptan	F ₃ CSCl	136.5200	-0.7000		
2,2 difluoro propane	(CH ₃) ₂ CF ₂	80.0800	-0.4000	-104.8000	0.9205
nitro pentafluoro ethane	CF ₃ CF ₃ NO ₂	165.0200	0.0000		
perfluoro 2-butene	CF ₃ CFCFCF ₃	200.0300	0.0000	-129.0000	1.5297
trans 2-butene	CH ₃ CHCHCH ₃	56.1200	0.9000	-105.5000	0.6042
1,1,1,2,2,3 hexafluoro propane	CH ₂ FCF ₂ CF ₃	152.0400	1.2000		
perfluoro cyclobutene	C ₄ F ₆	162.0400	3.0000	-60.0000	1.6020
methyl bromide	CH ₃ Br	94.9400	3.6000	-93.6000	1.6755
bromo acetylene	BrCCH	104.9400	4.7000		
pentachloro benzyl chloride	C ₆ Cl ₅ COCl	312.8000	5.0000	87.0000	
hexafluoro 1,3 butadiene	CF ₂ CFCFCF ₂	162.0400	6.0000	-132.0000	1.5530
2-chloro 1,1,1 trifluoroethane	ClCH ₂ CF ₃	118.4900	6.9300	-105.5000	1.3890
dichloro fluoro methane or Freon 21	Cl ₂ CHF	102.9200	9.0000	-135.0000	1.4050
2-fluoro 1,3 butadiene	CH ₂ CFCFCF ₂	72.0800	12.0000		0.8430
acetyl fluoride	CH ₃ COF	62.0400	20.8000		1.0020
1,2 dichloro 1,2 difluoro ethylene	ClCFClCFCl	132.9200	21.1000	-130.5000	1.4950
1-nitro heptafluoro propane	CF ₃ CF ₂ CF ₂ NO ₂	215.0300	25.0000		
neopentyl chloride	(CH ₃) ₃ CCH ₂ Cl	106.6	84.3000	-20.0000	0.8660

ADSORPTION PHENOMENA IN AEROGEL BED – There are many possible adsorption isotherm models that can be used to predict the coverage of high surface area materials by and adsorbing molecule from either gas or liquid phases. One of the most widely used and best known is the Langmuir isotherm, that will be used as the basis of discussion in this proposal. However, during execution of the work, other isotherms will be explored to determine the most appropriate for modeling refrigerant adsorption on the various types of aerogels that will be explored.

In this discussion, it is assumed that the fractional coverage of active sites on the surface of the aerogel by adsorbed refrigerant can then be calculated from the Langmuir parameter and the gas-phase chemical activity of the species being adsorbed. The chemical activity is proportional to gas-phase above the surface where adsorption is occurring. Langmuir adsorption isotherms have been predicted for various compounds, including iso-butane on zeolites, as a function of pressure and temperature. In the case of iso-butane adsorbed on zeolite, predictions were based upon Langmuir parameters determined from the regression analysis of published data. In this specific case (isobutene on zeolite), temperature changes induced by solar heating appear to be insufficient to cause enough change in surface coverage and gas-phase pressure to drive a practical refrigeration cycle. Similar predictions have been made with optimized combinations of refrigerant and adsorption media (optimum specified in terms of predicted Langmuir parameter). In this optimized case, temperature changes induced by solar heating do appear to be sufficient to cause enough change in surface coverage and gas-phase pressure to drive a practical refrigeration cycle.

Adsorption of refrigerant on the surface of the aerogel (or other adsorption media) may obey the Langmuir adsorption isotherm. The Langmuir parameter for the i^{th} species (K_i) is defined by the Gibbs free energy of adsorption, the universal gas constant, and the absolute temperature. The fractional coverage of active sites on the surface of the aerogel by adsorbed refrigerant can then be calculated from the Langmuir parameter and the gas-phase chemical activity of the species being adsorbed (a). The chemical activity is proportional to gas-phase above the surface where adsorption is occurring. In cases involving multi-component refrigerants, refrigerants compete for available active sites, in accordance with the following modified adsorption isotherm.

$$K_i = \exp\left(\frac{-\Delta G_i^0}{RT}\right) \quad \frac{\theta}{1-\theta} = a \exp\left(\frac{-\Delta G_{ADS}}{RT}\right) \quad \theta = \frac{a \exp\left(\frac{-\Delta G_{ADS}}{RT}\right)}{a \exp\left(\frac{-\Delta G_{ADS}}{RT}\right) + 1} \quad \theta_i = \frac{K_i a_i}{1 + K_i a_i + K_j a_j}$$

PREDICTED PERFORMANCE FOR ADSORPTIVE REFRIGERATION CYCLES – The Langmuir parameters for the adsorption of normal- and iso-butane on zeolites have been determined as a function of temperature, and regression analysis have been used to establish the temperature dependence, based upon published data. Preliminary analyses based upon this isotherm data indicate that in the specific case of iso-butane on zeolite, the temperature changes induced by solar heating may be insufficient to cause large enough change in surface coverage and gas-phase pressure to drive practical refrigeration cycles. However, additional work is required to be certain.

The predicted Langmuir adsorption isotherm for a better refrigerant and adsorption-medium combination at various temperature levels are shown in Figure 6a. These predictions were based upon, with the free energy of adsorption and pre-exponential for calculation of the Langmuir parameter summarized below. One possible refrigeration cycle is shown as an overlay on the isotherm. The legend gives predictions for various temperature levels (°F). In this more optimal case, temperature changes induced by solar heating do appear to be sufficient to cause enough change in surface coverage and gas-phase pressure to drive a practical refrigeration cycle. For a carbon aerogel with a demonstrated active surface area of 3,125 square meters per gram, and assuming a monolayer coverage of iso-butane, a mass loading of approximately 0.6 grams of isobutene per gram of aerogel is estimated. By using materials with even higher surface areas, loadings of 1 gram per gram or better may be possible.

One possible refrigeration cycle, and probably not the most optimal, is shown in Figure 6b. The path from F to A represents condenser operation between 175°F and 140°F, removing superheat and the latent heat of vaporization from the refrigerant. Then, the path from A to B represents the expansion of refrigerant, with partial condensation in the evaporator, which is assumed in this example to be operating at 10°F. The adsorption bed operates along the path, between points E and F. Clearly, these are relatively crude calculations that do not fully account for the transient nature of the system. A transient model will be developed during the project.

An optimized carbon aerogel adsorption medium is assumed with 3,125 square meters per gram and an assumed mass loading of isobutene refrigerant (R600a) of 0.6 grams per gram at saturation. While the exact details of this specific adsorption isotherm are not known, a temperature-dependent Langmuir parameter was estimated with an assumed free energy of adsorption of approximately 45,000 Joules per mole, and a representative pre-exponential. The adsorption bed is assumed to discharge iso-butane at 175°F. The condenser removes superheat and the latent heat of vaporization at 140°F and a pressure of 127 psi. The evaporator is assumed to operate at 10°F and 14.6 psi. For a 10-ton cooling unit, with an assumed operation of 8-hours per day, for 120 days per year, the following estimates have been made and are summarized in Table 3.

Table 3 – Estimated mass loading iso-butane on of high-surface-area adsorption beds.

	Low Area	High Area	Low Loading	High Loading
Material	m ² /g	m ² /g	g/g	g/g
Activated Carbon	100	1500	1.93×10 ⁻⁰²	2.90×10 ⁻⁰¹
Carbon Aerogel	1500	3125	2.90×10 ⁻⁰¹	6.03×10 ⁻⁰¹
More Advanced Materials	6000	7000	1.16×10 ⁺⁰⁰	1.35×10 ⁺⁰⁰

Note: This assumes that the adsorbate is iso-butane with a molecular weight of 58.12 grams per mole, and surface coverage at saturation of about 2×10^{14} molecules per square centimeter.

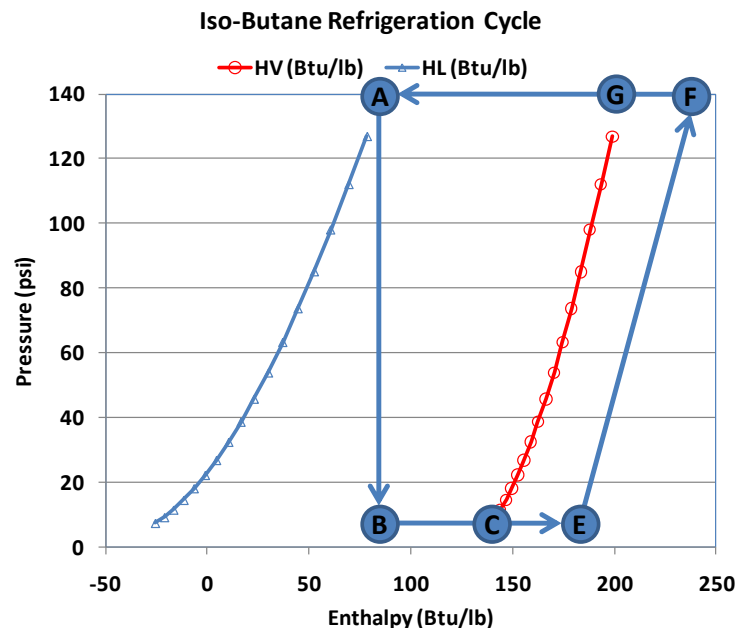
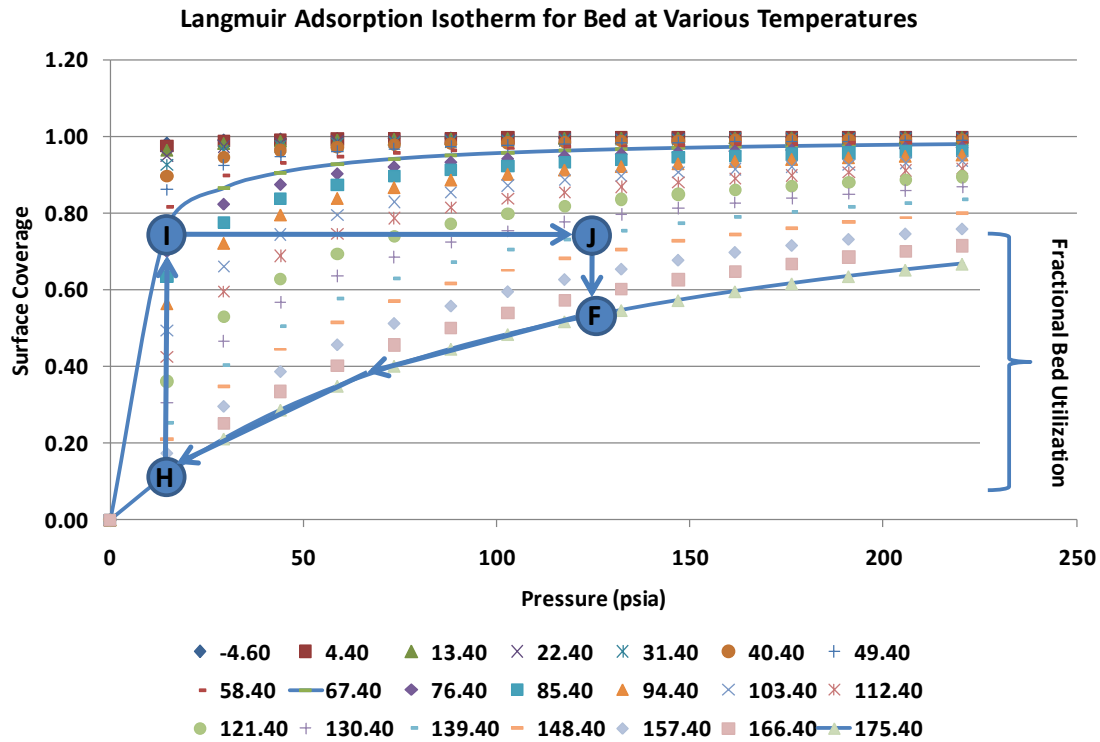


Figure 6 – (a) Predicted Langmuir adsorption isotherms for more optimal combination of refrigerant and adsorption media, with each data series plotted representing the temperature in Fahrenheit, and one possible refrigeration cycle shown on left; and (b) hypothetical iso-butane refrigeration cycle depicted on a pressure-enthalpy chart shown on right.

Significance of Proposed Effort with Respect to FOA Requirements

The team will produce a solar-driven adsorption-based refrigeration system that directly converts solar heat to the work of compression necessary to drive the cool system. The system will use high-surface-area aerogel adsorption beds, which reduce the system's size footprint, for ease of installation. The system will have the ability to use refrigerants other than CFCs, which damage the ozone layer. Exceptional thermal insulation will be provided through our proven injection-molded silica aerogel, which has the best heat transfer resistance of any known engineered material, and will therefore help control heat leakage in the refrigeration and air conditioning system, increasing the overall efficiency. This, combined with optics to enhance solar concentration, will enable operation in colder climates. The system will have no moving parts and require no lubricants, for exceptional ease of maintenance and low operating costs. It will have a hermetically sealed pressure envelope containing the refrigerant, thus minimizing the probability of refrigerant leakage from the system and eliminate the need for periodic charging of the system with makeup refrigerant. Eliminating the need for a compressor, which accounts for roughly 80% of the energy costs of conventional air conditioning systems, the proposed solar-driven system will drastically reduce cooling costs and greatly reduce carbon output. Long-term reduction in the price premium is assured by future improvements in materials and manufacturing processes, per-unit cost savings at industrial-scale fabrication, and other improvements such as designing the system to cycle multiple times per day. Commercialization will be helped by the team's experience with the industrial-scale manufacturing of aerogels and through close coordination with LLNL's technology transfer organization from the early stages. In view of the relative simplicity of the system's components, along with America's intellectual property in aerogels and other nanostructural materials, the system could be manufactured domestically and marketed globally as a next-generation green building technology, for excellent **job-creation** prospects.

ENERGY BENEFITS – A hypothetical 10-ton cooling unit—which would be appropriate for a 10,000-ft² commercial low-rise building—operating 8 hours per day for 120 days per year is assumed. The solar-driven cooling system could theoretically save as much as 80% on cooling energy costs by eliminating the need for a compressor, which in general accounts for 80% of a conventional cooling system's energy costs. The proposed system would only require air-handling (i.e., fan) energy costs, which account for the remaining 20%. For a 10,000-ft² building, this amounts to a predicted energy savings of \$4,570 per year, assuming a compressor efficiency of 55% and a cost of electricity of \$0.10 per kilowatt-hour. Even allowing for factors such as auxiliary power use on cloudy days, the system should **reduce cooling energy costs by 30–60%** over conventional air conditioning systems. The **system's estimated EER is 30** because of the use of solar rather than electrical energy and the direct conversion of solar energy to the work of compression.

An estimate for the energy and carbon savings achievable using this technology is found by multiplying the total U.S. values by a reduction-multiplier equal to the U.S. target market fraction (80%) multiplied by the market penetration (12%) multiplied by the fraction of energy replaced by the new technology (100% space cooling, 75% water heating, 50% space heating). This results are shown in Table 4. The total expected U.S. savings is 0.73 quads/yr and 57 million metric tons of carbon per year.

Table 4 – Concept of Operations of Hypothetical Carbon-Aerogel Based HVAC Systems.

Concept of Operations (Con-Ops)				
Scenario	Description	1. Single Bed & Ballast Volume	2. Two Beds & Multiple Cycles	3. Two Beds & Multiple Cycles & Optimized HE
Refrigeration	Tons	10	10	10
Refrigeration	Btu/hr	120,000	120,000	120,000
Refrigeration	Btu/min	2,000	2,000	2,000
Refrigeration	Watts	35,170	35,170	35,170
Assumed Duty Cycle	hours/day	8	8	8
Assumed Duty Cycle	days/year	120	120	120
Assumed Duty Cycle	hours/year	960	960	960
Parallel Adsorption Beds	Number	1	2	2
Frequency	cycles/day	1	16	16
Circulating Refrigerant				
Satd. Liquid Evaporator	Btu/lb	-11.50	-11.50	-11.50
Satd. Vapor Evaporator	Btu/lb	147.00	147.00	147.00
ΔH_{vap}	Btu/lb	159	159	159
Entering Evaporator	Btu/lb	78.50	78.50	4.50
Evaporated Refrigerant	lb/hr	757	757	757
Evaporated Refrigerant	lb/day	6,057	6,057	6,057
Evaporated Refrigerant	kg/day	2,750	2,750	2,750
Quality of Refrigerant	XL	0.43	0.43	0.90
Total Refrigerant Flow	(lb/day)/XL	14,015	14,015	6,737
Total Refrigerant Flow	(kg/day)/XL	6,363	6,363	3,059
Fixed Adsorption Bed of Aerogel				
Specific Area	m ² /g	3,125	3,125	3,125
Saturation Loading	g/g	0.60	0.60	0.60
Bed High Temperature	°F	175	175	175
Bed High Pressure	Psi	127	127	127
Bed Low Coverage	Fractional	0.54	0.54	0.54
Bed Low Temperature	°F	10	10	10
Bed Low Pressure	Psi	15	15	15
Bed High Coverage	Fractional	0.97	0.97	0.97
Differential Coverage	Fractional	0.43	0.43	0.43
Differential Loading	g/g	0.26	0.26	0.26
Required Media	Kg	24,524	3,065	1,474
Density Adsorption Media	kg/L	0.50	0.50	0.50
Volume of Adsorption Bed	L	49,048	6,131	2,947
Volume of Adsorption Bed	m ³	49.05	6.13	2.95
Dimension of Bed	Meter	3.7	1.8	1.4
Dimension of Bed	Foot	12.0	6.0	4.7
Work of Compression				
Work Required	Btu/lb	51	51	51
Work Required	Btu/day	714,745	714,745	343,579
Work Required	Btu/year	85,769,343	85,769,343	41,229,474
Work Required	Wh/lb	15	15	15
Work Required	kWh/day	209	209	101
Work Required	kWh/year	25,137	25,137	12,083
Performance Metrics				
Refrigeration Effect	Btu/lb	121	121	195

Heat of Compression	Btu/lb	51	51	51
Coefficient of Performance	Btu/lb	2.36	2.36	3.81
EER		~ 30	~ 30	~ 30
SEER		TBD	TBD	TBD
Cost Savings Over Comparable Mechanical Compression System				
Mechanical Compressor	Efficiency	0.55	0.55	0.55
Mechanical Compressor	kWh/year	45,703	45,703	21,969
Electricity Cost	\$/kWh	0.10	0.10	0.10
Electricity Cost	\$/year	\$4,570	\$4,570	\$2,197

ENVIRONMENTAL BENEFITS - This technology will **reduce global warming potential** by reducing carbon released by electricity generation with fossil fuels; **reduce ozone destruction** by operating on non-CFC refrigerants; **reduce pollutants and wastes** by being hermetically sealed (so that no coolant escapes), by not requiring recharging (which is when much coolant is accidentally released) or lubricants, and by having no moving parts to wear out and be replaced; and **improve recyclability**, as the refrigerant can be reused as it is not dirtied by lubricants, which are not needed. Table 5 shows energy and carbon savings based upon projections by the U.S. Department of Energy (<http://buildingsdatabook.eren.doe.gov/>) (<http://www.eia.doe.gov/>).

Table 5 – Total Energy and Carbon Savings with Aerogel Technology Proposed to ARPA-E.

Building Energy Use	Energy Source for All Buildings 2006 (Quads)*			Total Carbon 2006 (Million Metric Tons/yr)*	Target Market Size (% Total)**	Expected Market Penetration 10+ yrs. (%)	Efficacy per Building (%)	Total Market Multiplier
	Natural Gas	Oil	Electric	Total				
Space Cooling	0.02		1.54	290	0.80	0.12	1.00	0.10
Water Heating	1.63	0.15	0.58	210	0.80	0.12	0.75	0.07
Space Heating	4.31	0.84	0.53	420	0.56	0.12	0.50	0.03
Total	5.96	0.99	2.65	920				
Total Savings	0.57	0.07	0.09	57				

ECONOMIC IMPACTS – The U.S. has controlling intellectual property on aerogels, which would give the country a competitive advantage over foreign manufacturers. Aerogel-based solar cooling is positioned to become a linchpin next-generation technology that U.S.-based producers could manufacture for the global market. Thus this technology represents a nanomaterials-based strategy to anchor appliance manufacturing in the U.S. and would be key part of clean-energy portfolio that could make U.S. a global leader in green building technology. In short, this is a transformational technology with the potential for globally game-changing impact. This technology could drive the foundation of multiple startups to manufacture specific materials and components and to assemble and market the final products. Because of the system's relatively simple construction (e.g., no moving parts), manufacturing could be sited in relatively "low tech" communities. Beyond commercial buildings, manufacturers could also market to other air-cooling applications, including cooling homes and passenger compartments in cars, trucks, commercial ships, and airplanes; cooling high-performance computers and electronics; and cooling advanced energy conversion and storage devices, including batteries.

Milestones

By executing the tasks outlined in the *Approach* section, the following milestones will be achieved during this project. Two critical GO/NO-GO milestones have been identified:

- Successful demonstration of reversible refrigerant adsorption on single bench-scale bed of carbon aerogel (or higher surface alternative if found) by the end of FY1 Q4.
- Successful use of single bench-scale bed of carbon aerogel (or higher surface alternative if found) to force refrigerant through expansion valve, with demonstrated refrigeration effect by the end of FY2 Q4 (final quarter of seedling).
- Successful demonstration of reversible refrigerant adsorption on larger parallel bench-scale beds of media for commercialization – work beyond scope of seedling.

Table 6 – Tasks, Deliverables, and Milestones for Initial Seedling Project

	FY1				FY2			
Tasks, Milestones & Deliverables	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1 – Produce Initial UHS-CA								
Task 2 – Determine Adsorption Isotherms								
Task 3 – Produce Additional UHS-CA								
Task 4 – UHS-CA Production QA								
Task 5 – Computer Aided Design								
Task 6 – Design Single-Bed Components								
Task 7 – Build Single-Bed System								
Task 8 – Test Single-Bed System								
Task 9 – Calibrate Computer Model								
Task 10 – Design Multiple-Bed System								
Task 11 – Test Multiple-Bed System								
Task 12 – Incorporate Aerogel Insulation								
Task 13 – Begin Commercialization								

Performance Team

The team includes Lawrence Livermore National Laboratory (LLNL) and Ocellus Incorporated, a spin-off of LLNL involved in the commercial manufacture of various nanostructural materials, including aerogels.

Lawrence Livermore National Laboratory (LLNL)

Livermore scientists and engineers developed a patented, licensed, and award-winning aerogel-based process that provides many of the advantages of ion exchange for water purification, but without the need for chemical regeneration and the associated secondary waste stream. The adsorption media in this innovative system was electrically regenerated. Two regenerable adsorption beds operated in a potential-swing mode. A similar strategy could be used to achieve continuous cooling in the proposed system. This system was designed, built, and successfully demonstrated by investigators, who received an R&D100 Award for their efforts. This technology was licensed three times, and a miniaturized version system is the subject of a new CRADA. An optimized prototype system will be installed and tested in this thermally isolated HVAC testing facility at LLNL. Solar collectors and adsorption–desorption beds can be installed on top of the adjacent containers.

Chemical Sciences Division – The Chemical Sciences Division (CSD) conducts R&D at the intersection of chemical and nuclear science in support of LLNL's missions. CSD personnel provide expertise in organic, inorganic, analytical, computational, nuclear, and environmental chemistry, as well as engineering and physics, to solve problems in stockpile stewardship and other national security programs. The CSD is internationally recognized as a leading center for the design and fabrication of porous materials, specifically aerogels and related sol-gel materials, and is uniquely positioned to fabricate both the high-surface-area aerogel adsorbents and the insulating materials for this effort. **Condensed Matter and Materials Division** – CMMD is the center of LLNL's integrated and comprehensive condensed-matter physics and materials science core competencies. The division provides innovative and responsive science in support of the programs and performs discovery-class science ahead of the programs. Scientists in CMMD play leadership roles in the scientific community in these key and emerging areas of condensed-matter and materials science. **Engineering Technologies Division** – ETD staff provides advanced analysis, research, test, and design capabilities across many engineering and physical sciences. Notably ETD includes staff dedicated to the thermal-fluids and materials sciences. ETD frequently manages large development projects for external customers, including many for DOE. Projects are managed using earned-value metrics, and engineering practice is subject to established guidelines for quality and safety. Many tools are applied as appropriate, including thermodynamic system models, computational fluid dynamics, and finite element methods and experimental verification. Recent related projects include (1) HVAC modeling of chemical processing facilities, (2) thermodynamic and process analysis of an aerogel supercritical extractor, (3) thermodynamic and process analysis of a tritium processing system, (4) gas–solid chemical adsorption and diffusion analysis, (5) diesel combustion and byproduct analysis, and (6) thermal design of cryogenic instrument packages. **Project Management Engineering and Construction Department** – The PMEC Department provides engineering design, estimating, management services for LLNL construction projects, including general plant projects, capital equipment and project, line item projects, and special facilities projects. The division's expertise spans the full spectrum of industrial building needs, including HVAC and other systems.

Industrial Partnerships Office – The IPO—LLNL's conduit to the private sector—helps Laboratory scientists collaborate with industry to achieve Livermore's objectives. IPO has extensive experience protecting and commercializing intellectual property, is recognized as having the **highest earned royalty income of all national laboratories**, and launches many industrial collaborations every year.

Joseph C. Farmer – Senior Scientist of the Condensed Material and Materials Division. With a Ph.D. in chemical engineering, Joe has more than 30 years professional experience in research and development, more than 170 publications, and numerous patents and awards, including an R&D 100 Award for processes for the efficient separation of ionic solutions with bipolar membrane electrodialysis and carbon aerogel foams. Most recently, he led the DARPA-DOE High-Performance Corrosion-Resistant Materials Program. Joe will serve as PI for this project. His availability is up to 100% if required. **Wayne O. Miller** – Leader of LLNL's Thermal Fluids Group in the Engineering Technologies Division. He has a Ph.D. in mechanical engineering, and his technical focus is on thermal-fluid systems and numerical analysis. Wayne will function a co-PI and subject-matter expert. His availability is up to 33%. Staff are also available as needed. **Joe H. Satcher, Jr.** – Program leader in the Physical and Life Sciences Directorate and leader of the Advanced Materials Synthesis Group, in CSD. Joe has over 28 years of experience in synthetic and polymer chemistry as well as sensor design. In his 11 years as AMS group leader, Joe has successfully managed a number of different projects, including a biosensor project that earned his team the DOE Bright Light Award and the DOE Federal Laboratory Consortium Award for Excellence in Technology Transfer. **Theodore F. Baumann** – Staff scientist in CSD with over 20 years of experience in organic and inorganic synthesis. He is currently leading a project in the DOE H2 Program focused on new materials for hydrogen storage. He is an expert in the design of porous and nanostructured materials. **Robert H. Simonds** – Mechanical engineer in the PMEC Department with extensive HVAC experience. He has been a registered professional engineer since 1979 and has worked at LLNL for 26 years, during which time he has designed HVAC and other building systems for industrial facilities, laboratories, and office spaces. **Robin Miles** – Senior Engineer, LLNL Nanotechnology Center. She holds a M.S. in mechanical engineering from Stanford, as well as an M.B.A. from UC Berkeley. She has unusual expertise in the fabrication of ceramic components for microwave devices, which will be exploited in the development of the solid-state electrolyte-separator necessary for the success of this project. She also has experience in physical and chemical vapor deposition.

Ocellus Incorporated

Ocellus Inc. is a California corporation formed in 1996 by Dr. Michael Droege (see U.S. Pat. 5,395,805 in section on LLNL intellectual property, for example) to lead commercialization of nanofoams materials. These materials are a special class of foams where the air spaces and solid matter are so small that they are invisible to the eye; thus these materials possess unique properties important for a range of applications. A variety of nanofoam materials are available including silica (glass), alumina, phenolic, and carbon. Ocellus focuses on high-value technology markets, emphasizes R&D to discover new materials, developing new processing techniques, and advanced engineering. Ocellus creates high-value engineering concepts and prototypes. Business activities include the manufacture and sale of nanofoams through a distributor, contract R&D, and out-licensing of proprietary technology. Ocellus' has a 4,000 square foot laboratory facility dedicated to R&D and production. Ocellus possesses all equipment needed to perform a wide range of materials preparation, processing, and testing.

Related Work

Ocellus has been active in developing novel aerogel and nanophase foams and composites for a variety of applications that center on thermal management. The following summarizes some of this work:

- Ocellus teamed with Boeing to develop an aerogel/fiber high temperature insulation material for NASA.
- For the Air Force, Ocellus demonstrated an aerogel composite insulation for high velocity air craft.
- For the Navy, Ocellus developed a low-cost sprayable aerogel-based insulation material.
- With Navy support, Ocellus is currently scaling-up this process to begin commercialization of this technology.
- Batch pilot facility has been constructed.
- Ocellus is beginning production of 100 kg batches of carbon nanofoam for use in electronic applications.

Facilities/Equipment

Ocellus maintains a facility in Livermore, California. This location is a 4,000 square foot laboratory facility dedicated to the R&D and production of materials. The facility is designed for chemical handling and includes benches, fume hoods, and chemical storage areas. Ocellus possesses all equipment needed to perform a wide range of materials preparation, processing, and testing. This equipment includes: supercritical extraction systems, horizontal flow curing/drying ovens, 1200°C pyrolysis furnaces, wide assortment of analytical and test equipment, and light machining equipment.



Figure 7 – Ocellus Incorporated facilities in Livermore, California, with capability of producing large quantities of carbon aerogels, and characterizing the materials produced.

Transition and Commercialization Strategy

Commercialization Strategy

Led by the Industrial Partnerships Office, LLNL will employ a three-point plan to commercialize the proposed cooling system. The Laboratory is already successfully using this strategy for other technologies, including its “clean tech” portfolio.

OPTIMIZE DEVELOPMENT – We will develop and protect intellectual property as the technology matures and interact early with domain experts to avoid costly and time-consuming redesign; with potential industrial users during the early prototype stage to understand sector-specific needs, system integration issues, and building codes and to analyze life-cycle investment and costs and propose incentives for commercial builders, landlords, and tenants; and with code-setting bodies during the late prototype stage to ensure the proper and rapid deployment of the technology. We will also use the appropriate tools for measurement and verification of energy savings.

INTRODUCE IN COLLABORATION WITH USERS AND POTENTIAL LICENSEES – The team can use multiple clean technology beta-test sites co-developed with local industry in different climate zones to mature technologies and promote adoption. There, we will collect long-term data on energy use, robustness, and cost; showcase the use of the technology to educate users and encourage demand and adoption; demonstrate synergies with other clean technologies; train builders regarding the installation of the system and its integration into existing systems; maximize DOE investment by involving potential licensees who provide matching contributions; and develop channels of commercialization through collaboration with potential licensees. LLNL plans to install the final optimized system first at the Arc of Hilo, in Hilo, HI, where two other “clean technologies” are already slated to be beta-tested—another solar thermal scheme and a flywheel-based electromechanical battery technology. The Arc of Hilo has an 18,000-ft² warehouse where local farmers can develop higher-value food products. Arc of Hilo Director Mike Gleason plans to make the building “green” using the aforementioned two technologies. Says Gleason, “We think working with the Lab and these technologies are a tremendous fit. It will allow us to create these job opportunities with much lower energy consumption.” The proposed HVAC system promises to be another key component of this mission. Another test site will be secured in a Mediterranean climate (Livermore, CA). This site will simulate the requirements of a high-demand cooling application, a computer data center. A third (cool-weather) site will be chosen in early 2010.

MAXIMIZE COMMERCIALIZATION THROUGH MULTIPLE CHANNELS – In this stage, we will collaborate with and educate licensees and industrial users of the technology as soon as possible, preferably during prototype development, but at least during beta testing; co-develop mutual understanding of the market channels with licensees and industrial partners; maximize market penetration by minimizing early overlap between market sectors served by various licensees; use licensing strategies that reflect the business model of the licensee and achieve mutual benefit; select and monitor aggressive but achievable licensee performance requirements; and maintain continued collaboration with licensees, supporting cooperation among licensees with complimentary technologies.

Market Potential

The DOE estimates the total primary energy consumption for commercial buildings was 10.72 quadrillion BTU (quads) in 1983, compared with 14.74 quads for the residential sector. According to the DOE Building Technologies Program, 40–60% of the energy used in U.S. commercial (and residential) buildings is for HVAC, creating massive potential for energy savings with a system that could cut cooling energy use by at least 30–60%. Initial vertical segments in the commercial building market include government and commercial office buildings; government facilities such as prisons, military bases, and schools; hotels and resorts; farming, wineries and other rural facilities; and general light industrial offices (e.g., printers and clothing makers).

MARKET TRENDS – According to the market assessment group Frost and Sullivan, “Even though renewable energy technologies integrated with HVAC systems are presently holding a negligible share in the U.S. market, they are poised to gain significant momentum over the next decade. This trend is driven by factors such as the demand to reduce carbon emissions, legislation, and expected cost competitiveness. Regulatory bodies, environmental consciousness, price, and efficiency-sensitive customers are positively influencing the technological capabilities and competitive structure of the HVAC equipment markets.” Another market assessment group, Reportlinker, expects U.S. demand for HVAC equipment to increase 4.5% annually through 2013 to \$17 billion, buoyed by an expected rebound from the current sluggish economy. Two market segments exist for commercial HVAC systems: new buildings and retrofitting. Although the retrofit market is very conservative—most building owners do not consider a retrofit until the existing HVAC system is very old or has ceased to function—tax credits and other government stimulation are providing unprecedented interest and growth in both of these segments.

MARKET SHARE – As most of the technologies against which this technology will be competing are poorly developed, the potential of this technology is estimated conservatively at 10% of the existing green HVAC market share for commercial buildings. Although the prototypes have not yet been built, the fact that the technology is based on fundamentally sound physical principles and known manufacturing processes with low material costs leads the LLNL team to believe that the cooling system will not be more expensive than traditional technology after post-commercialization optimization (i.e., using lessons learned in the marketplace), and may even become less costly in the long term. The economic advantage of reducing energy costs by 30–60% or even as high as 80% is a major incentive and renders the economic potential of this technology very strong. The market potential of this technology could be quite large because the retrofitting of commercial buildings is in its infancy. If this technology is commercialized within the next 3 years, it could have a very strong market potential, which we can conservatively estimate at 15%. This is based on a payback period of about 3.4 years, which in turn assumes that the cost of the estimated amount of aerogel needed for a 10-ton cooling unit (24,524 kg) could be reduced to about \$34,000 per unit at commercial production levels.

Even if market penetration occurs slowly, even at half a percent per year, we can use the aforementioned market estimate of \$17 billion to forecast almost \$13 million in growth every year. Market strategies that will fortify and increase market penetration are (1) market promotion, e.g., in industry trade journals read by building managers and also by the mass media, given today's heightened interest in Earth-friendly technologies; (2) low-risk offers, i.e., limiting

the amount of retrofit that needs to be done by providing units that work seamlessly with existing HVAC systems; and (3) energy audit follow-ups.

POTENTIAL FOR SIZE REDUCTION – Estimates of the system size show that the adsorption–desorption beds of the system can be installed on a rooftop. Typical small commercial buildings require a 10-ton (35-kW) cooling system. Such a cooling unit would require an aerogel mass of about 24,000 kg for the simplest scenario, in which the beds are cycled only once per day. (This may seem large but is still the smallest possible volume of any adsorption-based scheme known.) The calculation for this scenario also assumes using iso-butane as the refrigerant and a 0.26 g/g differential refrigerant-to-aerogel loading (difference between loading during the adsorption and desorption phases). Assuming a solar efficiency of 50% and a 4 kWh/day fluence, which is typical in the eastern half of the U.S. (the Southwest has about twice this fluence available), the area need for the evaporation process is about 84 m², or about half of the roof area. Ways to reduce this size through better evaporator loading efficiencies up to a factor of two will be explored. Furthermore, it is theoretically possible to cycle a two-bed cooling system up to several times each day, thereby improving bed utilization. In this case, the required quantity of carbon aerogel for a 10-ton cooling unit would be reduced to approximately 3,000 kg, which would occupy adsorption–desorption beds only 6 m³ in size. Finally, more efficient use of heat exchanges between the refrigerant entering and exiting the evaporator will improve the refrigerant quality and could further reduce the aerogel requirement to less than 1,500 kg, or 3 m³.

TARGET GEOGRAPHIC MARKET – We assumed that the target market will about 80% of the continental U.S. for space cooling and water heating and about 56% of the continental U.S. for space heating, with the New England, the Mid-Atlantic, and the East North Central regions expected to exhibit a significantly lower likelihood of technology adoption because of lower available average solar fluence.

PRICE PREMIUM REDUCTION – The cost of the condenser and evaporator of the proposed system is comparable to that of current air-conditioning equipment, so the proposed system's main price determinant will be the cost of aerogel manufacturing. Carbon aerogel manufactured using current processes is estimated from previous work to cost \$5.76/kg when made with a resorcinol-formaldehyde critical-point extraction process or \$1.80/kg when made with a phenol-formaldehyde (PF) critical-point extraction process. The costs will be about 25% lower if a water-based extraction rather than a CO₂ critical-point extraction process is used. Thus, the cost for aerogel made with the PF water extraction process can be reduced to \$1.35/kg for this project. In addition, using a water-based solvent also enables an industrial-scale process using continuous mixing and flow-through furnaces, further reducing manufacturing costs. Finally, the quantity of aerogel required for the system can be reduced by cycling the system several times a day instead of just once. These cost reductions are summarized in Table 7.

Table 7 – Analysis of Possible Future Reductions in System Cost to Improve Position in Market

Cost strategy	Current method	Projected 10-ton aerogel cost	Future method	Cost reduction	New cost
Material replacement	Resorcinol-formaldehyde	\$100,000	Phenol-formaldehyde	66%	\$34,000
Fabrication scale-up	Small batch	\$34,000	Large, continuous	33%	\$22,000
Quantity reduction	1 cycle/day system	\$22,000	10 cycle/day system	70%	\$6,700
Total: 94%					

INTEGRATION WITH OTHER SYSTEMS FOR FURTHER ENERGY SAVINGS – System efficiency can also be greatly increased with only a slightly increased investment by using the system for heating in winter. In this configuration, the hot, desorbed refrigerant would go directly to an incoming air heat exchanger after going through the water heater stage. This represents a significant energy savings to the consumer. Additional system efficiencies could be gained by using a geothermal heat pump to pre-cool or pre-heat the incoming air. Payback periods for these systems are estimated to be 5–10 years. The major cost of the geothermal heat-pump system is the drilling to place fluid pipes underground to pump refrigerant through the moderate-temperature soil. To reduce this cost, we will also investigate techniques for increasing the efficiency of heat transfer between the working fluid and the ground, such as inducing chaotic advective flow or increasing soil thermal conductivity by injecting soil amendments near the conduit. Removing moisture from the air can also increase efficiencies. On a very hot, humid day, up to 100 g/m^3 of moisture could be removed from the air. In addition to increasing comfort, this airflow, at $5 \text{ m}^3/\text{min.}$, represents an additional 19 kW of power for condensation alone. Alternatively, the water in the humid incoming air could be adsorbed onto a water-sorbing bed, then desorbed through solar heating. A dual-bed setup similar to the one proposed for the desorbing refrigerant bed could be used for this process.

Additionality and Risk

Estimates of the system size show that the adsorption–desorption beds of the system can be installed on a rooftop. Typical small commercial buildings require a 10-ton (35-kW) cooling system. Such a cooling unit would require an aerogel mass of about 24,000 kg for the simplest scenario, in which the beds are cycled only once per day. (This may seem large but is still the smallest possible volume of any adsorption-based scheme known.) The calculation for this scenario also assumes using iso-butane as the refrigerant and a 0.26 g/g differential refrigerant-to-aerogel loading (difference between loading during the adsorption and desorption phases). Assuming a solar efficiency of 50% and a 4 kWh/day fluence, which is typical in the eastern half of the U.S. (the Southwest has about twice this fluence available), the area need for the evaporation process is about 84 m², or about half of the roof area. Ways to reduce this size through better evaporator loading efficiencies up to a factor of two will be explored. Furthermore, it is theoretically possible to cycle a two-bed cooling system up to several times each day, thereby improving bed utilization. In this case, the required quantity of carbon aerogel for a 10-ton cooling unit would be reduced to approximately 3,000 kg, which would occupy adsorption–desorption beds only 6 m³ in size. Finally, more efficient use of heat exchanges between the refrigerant entering and exiting the evaporator will improve the refrigerant quality and could further reduce the aerogel requirement to less than 1,500 kg, or 3 m³.

Commercialization risks include the high cost associated with establishing a manufacturing process for the proposed system. This risk will be mitigated by use of proven aerogel manufacturing processes; the rest of the system is comprised of traditional, off-the-shelf components. The regulatory climate could be slow to stimulate the replacement of existing HVAC systems. This risk will be mitigated by not relying on new regulations or incentive packages for market success. The cost of electricity could decrease, reducing the incentive to take on the risks associated with solar power. This risk will be mitigated by demonstrating more-than-adequate thermal storage for the HVAC system.

The cost of the condenser and evaporator of the proposed system is comparable to that of current air-conditioning equipment, so the proposed system's main price determinant will be the cost of aerogel manufacturing. Carbon aerogel manufactured using current processes is estimated from previous work to cost \$5.76/kg when made with a resorcinol-formaldehyde critical-point extraction process or \$1.80/kg when made with a phenol-formaldehyde (PF) critical-point extraction process. The costs will be about 25% lower if a water-based extraction rather than a CO₂ critical-point extraction process is used. Thus, the cost for aerogel made with the PF water extraction process can be reduced to \$1.35/kg for this project. In addition, using a water-based solvent also enables an industrial-scale process using continuous mixing and flow-through furnaces, further reducing manufacturing costs. Finally, the quantity of aerogel required for the system can be reduced by cycling the system several times a day instead of just once. The current technology readiness level (TRL) for this project is 3. By the end of the project, we expect to achieve TRL 6.

Technical risk will be further mitigated by LLNL's exceptional thermal modeling capability, which employs some of the world's most sophisticated thermal modeling codes, calibrated by a wealth of technical and scientific data from experiments. This approach will enable the rapid and cost-effective development of optimized designs, refrigerant selections, and concept of

operations prior to the fabrication of any prototype. Such codes can also be used to help quantify the effects of uncertainty and variability on predicted system performance, as well as on commercialization.

Manufacturing risk will also be mitigated with lessons learned from previous industrial-scale manufacture of aerogels (by LLNL licensee Aerojet in the mid-1990s) and by utilizing a current LLNL licensee, Ocellus, Inc., for the batch processing of aerogels at 100-kg scale. Commercialization risk will be minimized by leveraging the Laboratory's already appreciable experience and intellectual property portfolio in aerogel-based technologies, involving both the synthesis of these advanced materials, and the development of advanced processes that utilize these technologies. We will also proactively protect the intellectual property portfolio developed during development of the proposed cooling system to minimize the risk of losing the developed technology to overseas competitors. Commercial licenses will maximize the commercial

Commercialization risks include the high cost associated with establishing a manufacturing process for the proposed system. This risk will be mitigated by use of proven aerogel manufacturing processes; the rest of the system is comprised of traditional, off-the-shelf components. The regulatory climate could be slow to stimulate the replacement of existing HVAC systems. This risk will be mitigated by not relying on new regulations or incentive packages for market success. The cost of electricity could decrease, reducing the incentive to take on the risks associated with solar power. This risk will be mitigated by demonstrating more-than-adequate thermal storage for the HVAC system.

Management Plan

Project Management Team – Technical management of the team, as well as management of the overall project, will be conducted by the lead PI, Joseph Farmer, to whom co-PIs Wayne Miller, Ted Baumann, and Joe Satcher will report. This project management includes assuring close collaboration among the Condensed Matter and Materials Division, the Chemical Sciences Division, and the Thermal Fluids Group—all of which reside in LLNL's Science and Technology Principal Directorate—along with the Project Management Engineering and Construction Department and the Industrial Partnerships Office (which is funded by LLNL).

Adsorption Media and Candidate Refrigerants Screening Team – In the initial phase of the project, the lead PI will oversee the screening and selection of refrigerants in collaboration with Ted Bauman, Joe Satcher, and Wayne Miller. Those combinations of adsorption media and refrigerant determined to have acceptable performance, in regard to boiling point, latent heat of vaporization, adsorption capacity, free energy of adsorption, and reversibility, will be used as the basis of more detailed designs by the Thermal Modeling Team.

Aerogel Fabrication Team – Ted Baumann and Joe Satcher will guide the synthesis and characterization of the high-surface-area carbon aerogel and evaluation of refrigerant gas uptake and release in these materials. Joe Satcher will design and test the insulating aerogel materials.

Thermal Modeling Team – Wayne Miller, who leads LLNL's Thermal Modeling Group, will be responsible for thermal modeling of the proposed refrigeration cycle, including thermodynamic performance, system layout, and component design. The team will report directly to the PI.

System Design, Fabrication, Installation, and Testing Team – This team will comprise Joseph Farmer, Wayne Miller, and Bob Simonds and will form after the above-mentioned teams have completed their tasks. This team will design and fabricate operational prototypes and install and test them in a thermally isolated test facility, collecting and analyzing experimental performance data and then feeding that data back to the Thermal Modeling Team. This team will use the data to determine parameters in the thermal process model, then use that model to optimize the prototype system. After model calibration, additional data will be collected to enable validation of the process model, along with assessments of uncertainty and variability.

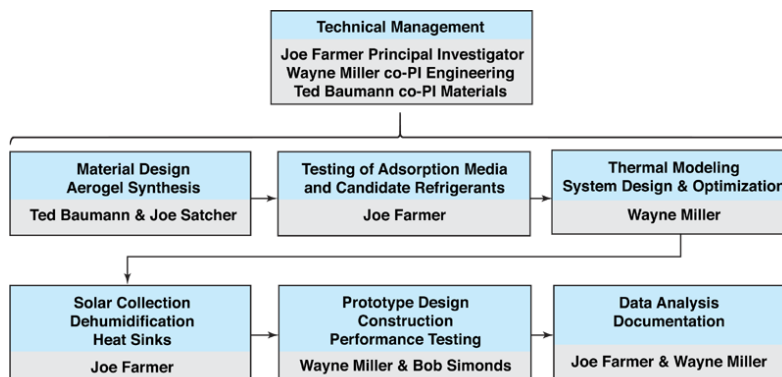


Figure 8 – Organizational chart for development of LLNL's solar-powered aerogel-based adsorptive air-conditioning system.

Budget Summary

Table 7 – Costs for ARPA-E Seedling Project Tasks

	FY1 FTE	FY2 FTE	FY3 FTE	Total FTE	FY1 \$K	FY2 \$K	FY3 \$K	Total \$K
ARPA-E					333	167		500
Matching					67	33		100
Total Effort & Cost	1.000	0.500		1.500	400	200		600
Task 1 – Initial Synthesis of Ultra High Surface (UHS) Carbon Aerogel (CA)	0.168	0.083		0.250	400	200		100
Task 2 – Determination of Adsorption Isotherms	0.125	0.000		0.125	67	33		50
Task 3 – Production Synthesis UHS-CA	0.250	0.125		0.375	50	0		150
Task 4 – Quality Assurance & Quality Control of UHS-CA Production	0.000	0.025		0.025	100	50		10
Task 5 – Computational Analysis & Design of System	0.013	0.025		0.038	0	10		15
Task 6 – Engineering Design of System & Components	0.025	0.025		0.050	5	10		20
Task 7 – Component Fabrication, Charging Adsorption Bed, Assembly & Installation	0.233	0.063		0.295	10	10		118
Task 8 – Performance Testing & Demonstration	0.188	0.155		0.343	93	25		137
Task 9 – Calibrated & Validated Computational Model for System Design								
Task 10 – Design & Optimization of Two-Bed Temperature-Swing Prototype								
Task 11 – Testing & Demonstration of Two-Bed Temperature-Swing Prototype								
Task 12 – High Performance Thermal Insulation Enhancement								

Note: Ocellus Incorporated of Livermore, California is providing at least 20% in-kind matching.

Appendix 1: Qualifications, Experience, and Capabilities

Joseph C. Farmer

Division Senior Scientist

Condensed Matter and Materials Division

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Education

Ph.D. Chemical Engineering, University of California, Berkeley, 1983

B.S. Chemical Engineering, Virginia Tech, Blacksburg, VA, 1977

Professional Experience

Lawrence Livermore National Laboratory (1987–present)

- Division Senior Scientist, Condensed Matter and Materials Science Division (2008–present). Led materials team for new ICF-based fusion energy initiative and principal investigator for related DOE NA-22 project. Consulted with federal agencies and others on advanced lithium-ion battery systems for various applications. Materials development for projects related to development of advanced energy conversion and storage, and rail guns.
- Principal Investigator and Project Manager, DARPA-DOE High Performance Corrosion Resistant Materials (HPCRM) Project (2003–2009). Responsible for the successful development of high-performance, corrosion-resistant, neutron-absorbing, amorphous-metal coatings that can be applied with various thermal spray processes. Led multi-institutional research team: DOE national laboratories, DOD laboratories, corporations and universities. Co-sponsored by DARPA Defense Science Office (DSO) and DOE Office of Civilian and Radioactive Waste Management (OCRWM) Office of Chief Scientist (OCS).
- Associate Program Leader, Nuclear Science and Systems Engineering Program, Global Security Principal Directorate (2006–2008). Developed materials for nuclear energy initiatives.
- Principal Investigator, DARPA Smart Surface Project (2005–2006). Responsible for the successful development of multifunctional coatings with special sensing capabilities.
- Chief Scientist, Acting Program Leader, Senior Scientist, Acting Technical Area Leader, Repository Science Program, Energy & Environment Directorate (1997–2004). Authored initial Waste Package Degradation Process Model Report (PMR – TDR-WIS-MD-000002 Rev. 0) and several of the original Analysis & Model Reports (AMRs – ANL-EBS-MD-000003 Rev. 0 and others) for proposed deep geological repository. Selection of engineering materials for spent nuclear fuel containers through testing and modeling. Defended waste package design at national level, including numerous briefings to the Under Secretary of Energy, the Nuclear Waste Technical Review Board and the Advisory Committee on Nuclear Waste.

- Principal Investigator and Team Leader, Process Development Team, Fissile Materials Disposition Program (1996–97). Responsible for process development supporting synthesis of new glass and ceramic waste forms, creation of ceramics processing laboratory (B241) for pressing and sintering ceramic waste forms, and the adaptation of induction-heated bottom-pour and tilt-pour furnaces for the production of prototypical glass waste forms.
- Laser Program Investigator (1996–97). LDRD investigator responsible for initially fielding experiments for the selection of protective optical coatings to prevent corrosion of silver flashlamp reflectors in National Ignition System.
- Group Leader and Principal Investigator, Electrochemical Processing Group, Materials Science and Technology Division (1992–1999). Author of several successful proposals for DOE Office of Basic Energy Science (OBES), DOD Strategic Environmental Research and Development Program (SERDP), United States Air Force (USAF), and DARPA DSO. Development and evaluation of large-scale electrochemical processes for the treatment of aqueous waste streams and water, novel thermoelectric thin-films, and models to predict the time-dependent reflectivity of large plated mirrors, accounting for atmospheric corrosion and protective optical coatings. Developed novel multilayer thermoelectric thin films and devices for direct energy conversion and cooling (work by research team received Award for Best Paper, International Thermoelectrics Conference, 1996). Initially sponsored by DOE OBES, subsequently Sponsored by DARPA DSO. Developed electrochemical process for removing ionic impurities from water, with minimal secondary wastes, using LLNL's carbon aerogel. Initially sponsored by SERDP, with subsequent sponsorship by USAF.
- Principal Investigator and Deputy Group Leader, Aqueous Processing Group, Environmental Technology Program (1990–92). Led R&D of electrochemical, photochemical, and thermochemical processes for the processing and treatment of mixed wastes.
- Principal Investigator, Deep Geological Repository Program (1987–1990). Initial materials selection for spent nuclear fuel and high-level waste containers to be placed in deep geological repository at Yucca Mountain.

PolyStor Corporation, Livermore, California (2000-2001)

- Director of Research and Development. [LLNL spin-off for high-volume manufacture of lithium ion batteries for the wireless communications industry, sponsored by National Institute of Standards and Technology (NIST) Advanced Technology Program (ATP)]. Led the scientific and technical team that included Argonne National Laboratory (ANL), Illinois Institute of Technology (IIT), Minnesota Mining and Metals Corporation (3M), and others. Responsible for winning, managing and executing NIST-sponsored ATP Project; developed electrode materials with high energy density; separators, electrolytes, and additive systems for inherently safe operation; high-integrity, light and soft packaging for advanced polymer-gel lithium ion batteries. Transitioned materials concepts to production. Established and operated the new Analytical Services Laboratory (SEM, EDS, FTIR, HPLC, GC, UV-Visible, TGA, DSC, BET, SSRT, CV, EIS). Recruited and trained technical staff. Investigated new battery materials and resolved technical problems facing productization. Assisted the company's chief technical officer and attorneys in the legal defense of intellectual property in this assignment.

Honors and Special Recognition

1999 Task Achievement Award – U. S. DOE CRWMS Management & Operating Contractor
 1996 Award for Best Paper, International Thermoelectrics Conference
 1995 R&D 100 Award
 1990 Silver Medal Award for Outstanding Paper in Plating Surface Finish – AESF
 1986 Norman J. Hackerman (Young Author) Award – Electrochemical Society
 1985 Gold Medal Award Plating Surface Finish – AESF
 1984 Boris and Renee Joffe Award for Best Paper, Interfinish '84, Jerusalem, Israel

Professional Society Membership

American Society of Mechanical Engineers
 Materials Research Society
 Electrochemical Society
 American Chemical Society
 American Society of Testing & Materials
 American Electroplaters & Surface Finishers Society, Research Board Member (prior)

Patents and Applications***Aerogel-Based Processes***

Method and Apparatus for Capacitive Deionization, Electrochemical Purification, and Regeneration of Electrodes, U. S. Pat. No. 5,954,937, September 21, 1999.

Method and Apparatus for Capacitive Deionization, Electrochemical Purification, and Regeneration of Electrodes, U. S. Pat. No. 5,428,858, June 20, 1995.

Means for Limiting and Ameliorating Electrode Shorting, U. S. Pat. No. 5,980,718, November 9, 1999.

Other

Indirect Detection of Radiation Sources Through Direct Detection of Radiolysis Products, Record of Invention IL-11,042, Lawrence Livermore National Laboratory, Livermore, CA; U.S. Pat. Appl. 11/292827, Filed December 1st 2005; PCT Appl. PCT/US06/44747, Filed November 16th 2006.

Detection of Corrosion and Warning of Chemical and Radiological Attack, Record of Invention IL-11,524, Lawrence Livermore National Laboratory, Livermore, CA; Provisional Appl. 60/711488, August 26th 2005, U.S. Pat. Appl. 11/293675, Filed August 23rd 2006; PCT Appl. PCT/US06/33183, Filed August 23rd 2006.

Paint for Detection of Radiological or Chemical Agents, Record of Invention IL-11,567, Lawrence Livermore National Laboratory, Livermore, CA; Provisional Appl. 60/712006, Filed August 26th 2005; U.S. Pat. Appl. 11/293657, Filed December 1st 2005.

Process for Making a Ceramic Composition for Immobilization of Actinides, U. S. Pat. No. 6,320,091, November 20, 2001.

Mediated Electrochemical Oxidation without Electrode Separators, U.S. Pat. No. 5,516,972, May 14, 1996.

Measuring Surfactant Concentrations in Plating Solutions, U.S. Pat. No. 4,812,210, Oct. 16, 1987.

Selected Publications (169 total)

Farmer, J.C., et al., "Capacitive deionization of NaCl and NaNO₃ solutions with carbon aerogel electrodes," *J. Electrochem. Soc.*, **143**(1): 159–169, (1996).

Farmer, J.C., et al., "Capacitive deionization of NH₄ClO₄ solutions with carbon aerogel electrodes," *J. Appl. Electrochem.* **26**: 1007–1018, (1996).

Farmer, J.C., et al., "Corrosion resistance of amorphous Fe_{49.7}Cr_{17.7}Mn_{1.9}Mo_{7.4}W_{1.6}B_{15.2}C_{3.8}Si_{2.4} coating: A new criticality control material," *J. Nuc. Tech.* **161**(2): 169–189, (2008).

Farmer, J.C., et al., "Corrosion resistance of iron-based amorphous metal coatings," *Proc. of ASME Pressure Vessels & Piping, Division Conference*, July 23-27, 2006, Vancouver, British Columbia, PVP2006-ICPVT11-93835.

Farmer, J.C., et al., "Corrosion resistance of thermally sprayed high-boron iron-based amorphous-metal coatings: Fe_{49.7}Cr_{17.7}Mn_{1.9}Mo_{7.4}W_{1.6}B_{15.2}C_{3.8}Si_{2.4}," *J. Materials Res.* **22**(8): 2297–2311, (2007).

Farmer, J.C., et al., "Corrosion resistances of iron-based amorphous metals with yttrium and tungsten additions in hot calcium chloride brine and natural seawater, Fe₄₈Mo₁₄Cr₁₅Y₂C₁₅B₆ and W-containing variants," *Critical Factors in Localized Corrosion 5, A Symposium in Honor of Hugh Issacs*, 210th Meeting of the ECS, Cancun, Mexico, 2006, in *Electrochem. Soc. Transactions*, **3**(31): 485–496, (2006).

Farmer, J.C., et al., "Electrosorption of chromium ions on carbon aerogel electrodes as a means of remediating ground water," *J. Energy and Fuels*, ACS, **11**(2): 337–347, (1996).

Wayne O. Miller*Thermal Fluids Group Leader*

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Education

Ph.D. Mechanical Engineering, Duke University, Durham, NC, 1990.

M.S. Mechanical Engineering, Duke University, Durham, NC, 1986.

B.S. Mechanical Engineering, University of Idaho, Moscow, ID, 1983.

Professional Experience**Lawrence Livermore National Laboratory (1996–present)**

- Thermal Fluids Group Leader, Engineering Technologies Division. Lead team of mechanical engineers with broad technical expertise in fluid dynamics, heat transfer, mechanics and chemistry; in a consultative, multidisciplinary environment, develop and lead new internal and external R&D projects and customer base, and perform project- and customer-oriented analysis tasks to support design efforts.

Kenetech Windpower, Inc., Livermore, CA (1994–1996)

- Aero-Structural Dynamics Analyst. Developed and improved in-house computational analytical capabilities and analyzed dynamic structural and aerodynamic loads of operating wind turbines; developed dynamic models of mechanical systems; designed airfoils using computational fluid dynamics; designed and analyze structural components using finite element techniques; developed new features for design software; correlated experimental and simulation data; evaluated and purchased MCAD software; ISO 9001 certified.

National Research Council, Mountain View, CA (1992–1994)

- Research Associate (NASA Ames guest researcher). Conducted R&D on advanced methods and algorithms for computational fluid dynamics and reducing numerical diffusion in three-dimensional Navier-Stokes calculations by combining high-order accuracy with adaptive gridding; developed MIMD parallel algorithm for solution of Poisson's equation using boundary elements and domain decomposition; implemented parallel algorithm on an Intel iPSC/860 using message passing.

Sterling Software, Palo Alto, CA (1991–1992)

- Research Specialist (NASA Ames contract employee). Conducted R&D on computational fluid dynamics methods for rotorcraft aerodynamics. Primary effort was the development of an adaptive resolution free wake model with vector code on a Cray Y/MP, providing order-of-magnitude efficiency gains. Preliminary research into dynamic computation of fluid/structure interactions, reduced-order models for large-scale computations, and CASE tools for scientific programming; provided support for full-scale wind tunnel experiments.

Professional Society Membership

American Society of Mechanical Engineers

American Institute of Aeronautics and Astronautics (prior)

American Helicopter Society (prior)

Patents

Rowland, M., Howard, D., Wong, J., Jessup, J., Bianchini, G., Miller, W., *Radiation detection system for portable gamma ray spectroscopy*, Patent No. 7064337, June 2006

Selected Publications (15 total)

Burks, M., Cork C., Eckels, D., Hull, E., Madden, N.W., Miller, W. , Goldsten, J., Rhodes, Williams, B., "Thermal design and performance of the gamma-ray spectrometer for the MESSENGER spacecraft," 2004 IEEE NSS/MIC/SNPS and RTSD, Rome, Oct. 2004.

Goldsten, J.O., Rhodes, E.A., Boynton, W.V., Feldman, W.C., Lawrence, D.J., Trombka, J.I., Smith, D.M., Evans, L.G., White, J., Madden, N.W., Berg, P.C., Murphy, G.A., Gurnee, R.S., Strohhahn, K., Williams, B.D., Schaefer, E.D., Monaco, C.A.; Cork, C.P., Eckels, D., Miller, W.O., Burks, M.T., Hagler, L.B., DeTeresa, S.J., Witte, M.C., "The MESSENGER gamma-ray and neutron spectrometer," *Space Sci. Rev.*, **131**(1–4): 339–391, Aug. 2007.

Kim, S., Lorente, S., Bejan, A., Miller, W., Morse, J. "The emergence of vascular design in three dimensions," *J. Appl. Phys.*, **103**(12), June 2008.

Miller, W. O., "Developing constructal theory as a tool for global security and sustainability," *Constructal Human Dynamics, Security and Sustainability*, NATO Science for Peace and Security Series E: Human and Societal Dynamics, **50**: 49–60, IOS Press, Amsterdam, 2008.

Miller, W.O., Darnell, I.M., Burke, M.W., Robbins, C.L., "Defining the envelope for sonic IR: Detection limits and damage limits," *Themosense XXV*, Orlando, FL, SPIE **5073**: 406–416, 2003.

Miller, W.O., et al., "Quantifying flaw characteristics from IR NDE data," *Themosense XXV*, Orlando, FL, SPIE **5073**: 417–425, 2003.

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Education

Ph.D. Inorganic Chemistry, University of California Davis, 1995

B. S. Organic Chemistry, University of California Davis, 1975

Professional Experience**Lawrence Livermore National Laboratory (1984–present)**

- Program Element Leader; Advanced Material Synthesis (1999–present)
- Staff Chemist, Chemistry and Chemical Engineering Division (1984–1999)

Tosco Corporation (1981-1984)

- Senior Chemist

Holly Sugar Corporation (1976-1981)

- Chief Chemist

Honors and Awards

Department of Energy Bright Light Award, awarded by Secretary of Energy Bill Richardson

Department of Energy Federal Laboratory Consortium (FLC) Award for Excellence in Technology Transfer, awarded by Secretary of Energy Spencer Abraham; April 2001

Selected Publications (132 total)

Pauzauskie, P.J., A. Jamshidi, J. K. Valley, J. H. Satcher Jr., M. C. Wu, “Parallel trapping of multi-walled carbon nanotubes with optoelectronic tweezers” *Appl. Phys. Lett.* 95, 113104 (2009).

Goksu, E.I., B. A. Nellis, W-C. Lin, J. H. Satcher, Jr., J. T. Groves, S. H. Risbud, M. L. Longo “Effect of Support Corrugation on Silica Xerogel–Supported Phase-Separated Lipid Bilayers”; *Langmuir*, 2009, 25 (6), pp 3713–3717.

Worsley, M.A., S. O. Kucheyev, J. H. Satcher, Jr., A. V. Hamza, T. F. Baumann, “Mechanically robust and electrically conductive carbon nanotube foams” *Appl. Phys. Lett.* 94, 073115 (2009)

Worsley, M.A., J. H. Satcher Jr., T. F. Baumann “Synthesis and Characterization of Monolithic Carbon Aerogel Nanocomposites Containing Double-Walled Carbon Nanotubes”; *Langmuir* 24 (2008) 9763 -9766.

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- Baumann, T.F., M. A. Worsley, J. H. Satcher, Jr. "High surface area carbon aerogel monoliths with hierarchical porosity" *J. Non-Cryst. Solids* 354 (2008) 3513–3515.
- Kucheyev, S.O., B. Sadigh, T. F. Baumann, Y. M. Wang, T. E. Felter, T. van Buuren, A. E. Gash, J. H. Satcher, Jr., and A. V. Hamza, "Electronic structure of chromia aerogels from soft x-ray absorption spectroscopy" *J. Appl. Phys.* 101, 124315 (2007).
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- Post-Doctoral Fellow (1997–1999)

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Selected Publications (over 50 total)

Worsley, M.A., J. D. Kuntz, P. J. Pauzaskie, O. Cervantes, J. M. Zaug, A. E. Gash, J. H. Satcher and T. F. Baumann “High Surface Area Carbon Nanotube-Supported Titanium Carbonitride Aerogels” *J. Matls. Chem.*, **2009**, *in press*.

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Michael Droege

Dr. Droege has more than 15 years of experience with nanoporous and mesoporous materials and a total of 20 years of materials research experience. He is one of the founders of Ocellus, Inc. and currently has direct responsibility for new product research and development for Ocellus. R&D activities are focused on organic and carbon nano-structure foams and aerogels for use in energy storage devices, sorptive processes, fuel cells, and thermal insulation.

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Selected Publications

1. Tran, T.D.; Lenz, D.; Kinoshita, K.; Droege, M.; "Effects of Processing Conditions on the Physical and Electrochemical Properties of Carbon Aerogel Composites", Mater. Res. Soc. Symp. Proc. 1998, 496, 607-611.
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Facilities and Equipment

SYNTHESIS LABORATORIES – The synthesis of the carbon adsorbents and the insulating aerogel materials will be performed in the chemistry laboratories within CSD. These laboratories are currently used for the synthesis and characterization of polymers, aerogels, and sol-gel materials and therefore contain the requisite equipment to support these efforts. The facilities include the autoclaves for conventional and rapid supercritical drying of the various aerogel materials as well as a full complement of needed laboratory equipment—fume hoods, high precision balances, ultrapure water, high-vacuum Schlenk manifolds, ovens, high-temperature furnaces, centrifuges, vacuum distillation and solvent stills, volumetric delivery systems, and pH, conductivity, oxygen, and ion selective electrode meters. In addition, these labs possess capabilities for gas adsorption studies and thermal conductivity measurements. Materials characterization facilities are also available onsite, including electron microscopy, x-ray diffraction, secondary ion mass spectrometry, elemental analysis, and soft x-ray spectroscopy.

INDUSTRIAL SCALE AEROGEL-BASED PROCESSES – Livermore scientists and engineers developed a patented, licensed, and award-winning aerogel-based process that provides many of the advantages of ion exchange for water purification, but without the need for chemical regeneration and the associated secondary waste stream (Figure 9). The adsorption media in this innovative system was electrically regenerated. Two regenerable adsorption beds operated in a potential-swing mode. A similar strategy could be used to achieve continuous cooling in the proposed system. This system was designed, built, and successfully demonstrated by Joe Farmer—the lead PI for this proposal—and his team at LLNL and received an R&D 100 Award. This technology was licensed three times, and a miniaturized version system is the subject of a new CRADA.

HVAC RESEARCH & TESTING FACILITY – This facility (Figure 10) was built to develop novel HVAC systems for DHS—contains sophisticated sensors, control systems, and heat exchangers that can be adapted for the proposed aerogel-based system. Our prototypes will be installed and tested inside this thermally isolated facility. The solar collectors and aerogel adsorption and desorption beds can be placed atop the adjacent containers.

CLEAN TECHNOLOGY DEMONSTRATION SITES – As part of a unique technology maturation effort for LLNL clean technologies, and in cooperation with LLNL's technical workforce development program, LLNL's IPO has developed the first of a group of technology prototyping sites, in Hilo, HI. This site can serve as a beta-testing site for the final optimized system.

COMPUTATIONAL DESIGN TOOLS – Before prototype construction, system optimization will be conducted computationally, using a broad range of design tools, including SINDA/FLUINT (thermal-fluid system design, performance, and optimization), STARCCM+ (computational fluid dynamics), TOPAZ (thermal finite-element analysis), NIKE, and ANSYS (structural finite-element analysis), and computational fluid dynamics and finite element analysis tools running on Livermore's parallel systems.

ADVANCED THERMAL ANALYSIS TOOLS – The Laboratory's world-leading thermal analysis technology will make it possible to optimize the system design before prototyping, thereby greatly reducing project risk.



Figure 9 – Award-winning aerogel-based process for the electrosorption of ionic impurities from water, demonstrating LLNL's ability to build industrial processes with novel nanostructural materials like those required for the refrigeration cycle proposed here.



Figure 10 – Thermal testing facility. The optimized prototype system will be installed and tested in this thermally isolated HVAC testing facility at LLNL. Solar collectors and adsorption

Appendix 2: Other Programmatic Issues

Cost Share

Ocellus Corporation will be provided with approximately \$150K in funding and will provide a 20% in-kind cost share for this project in the amount of \$100K. The cost share will be in the form of labor, equipment and facilities.

Appendix 3: Literature Cited

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Appendix 5: Intellectual Property

The Department of Energy (DOE) owned Lawrence Livermore National Laboratory (LLNL) has a dominant position in ultra high surface area carbon based foams needed for the further development of solar-driven adsorptive refrigeration cycles, including the HVAC system described in this proposal. The large portfolio of aerogel and aerogel-based process patents are listed in the following table. Licensing of this immense patent portfolio could be used to build an industry, create jobs and generate revenue.

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
8444	A	Richard Pekala	07/717581	04/11/91	5,081,163	01/14/92	Organic Aerogels from Polycondensation of Melamine with Formaldehyde
8444	B	Richard Pekala	07/684051	06/19/91	4,997,804	03/05/91	Melamine-Formaldehyde Aerogels
8477	B	Lawrence W. Hrubesh Thomas Tillotson John F. Poco	07/754349	09/05/91	5,275,796	01/04/94	Method for Producing Metal Oxide Aerogels Having Densities Less Than 0.02 g/cc
8477	D	Lawrence W. Hrubesh Thomas Tillotson John F. Poco Ian Melville Thomas	08/272432	07/07/94	5,409,683	04/25/95	Method for Producing Metal Oxide Aerogels
8625	B	Lawrence W. Hrubesh John F. Poco	07/972881	11/09/92	Attorney DOE / Notice of Abandonment 8/23/94		Stabilized Fuel with Silica Support Structure
8725	A	Thomas Tillotson Craig Wuest Coleman Johnson III	07/969084	10/29/92	5,416,376	05/16/95	Aerogel-Supported Filament
8743	A	Paul Coronado Lucy Hair Michael Droege	08/036997	03/25/93	5,395,805	03/07/95	Method for Making Monolithic Metal Oxide Aerogels

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
8818	A	Richard Pekala James Kaschmitter Steven Mayer	07/822438	01/17/92	5,260,855	11/09/93	Supercapacitors Based on Carbon Foams
8818	B	Richard Pekala James Kaschmitter Steven Mayer	08/036740	03/25/93	5,529,971	06/25/96	Carbon Foams for Energy Storage Devices
8818	C	Richard Pekala James Kaschmitter Steven Mayer	08/619393	03/20/96	5,789,338	08/04/98	Process for Producing Carbon Foams for Energy Storage Devices
8851	A	Joe Farmer Robert G. Hickman Francis T. Wang Patricia Lewis	07/933643	08/24/92	5,516,972	05/14/96	Mediated Electrochemical Oxidation of Organic Wastes Without Electrode Separators
8976	A	Richard Pekala James Kaschmitter Steven Mayer	08/057739	05/04/93	5,402,306	03/28/95	Aquagel Electrode Separator for Use in Batteries and Supercapacitors
9051	A	Richard Pekala James Kaschmitter Steven Mayer	08/183876	01/21/94	5,601,938	02/11/97	Carbon Aerogel Electrodes for Direct Energy Conversion
9060	A	Richard Pekala James Kaschmitter Steven Mayer Robert L. Morrison	08/041507	04/01/93	5,358,802	10/25/94	Doping of Carbon Foams for Use in Energy Storage Devices
9104	A	Joe Farmer	08/246692	05/20/94	5,425,858	06/20/95	Method and Apparatus for Capacitive Deionization, Electrochemical Purification, and Regeneration of

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
							Electrodes
9104	B	Joe Farmer	08/737687	11/15/96	5,954,937	09/21/99	Method and Apparatus for Capacitive Deionization and Electrochemical Purification and Regeneration of Electrodes
9154	A	Richard Pekala James Kaschmitter Steven Mayer John Herbert Fiekert	08/090881	07/08/93	5,336,274	08/09/94	Method for Forming a Cell Separator for Use in Bipolar-Stack Energy Storage Devices
9154	B	Richard Pekala James Kaschmitter Steven Mayer John Herbert Fiekert	08/229239	04/18/94	5,393,619	02/28/95	Cell Separator for Use in Bipolar-Stack Energy Storage Devices
9181	A	Richard Pekala James Kaschmitter Steven Mayer	08/041503	04/01/93	5,420,168	05/30/95	Method of Low Pressure and/or Evaporative Drying Of Aerogel
9184	A	Richard Pekala James Kaschmitter Steven Mayer Fung M. Kong	08/089119	07/08/93	5,508,341	04/16/96	Organic Aerogel Microspheres and Fabrication Method Therefor
9184	B	Richard Pekala James Kaschmitter Steven Mayer Fung M. Kong	08/586038	01/16/96	5,908,896	06/01/99	Organic Aerogel Microspheres
9260	A	Richard Pekala James Kaschmitter	08/110003	08/23/93	5,932,185	08/03/99	Method for Making Thin Carbon Foam Electrodes

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
		Steven Mayer Robert L. Morrison					
9291	A	Lawrence W. Hrubesh Gregory Sprehn John F. Poco Pamela H. Sandler	08/332285	10/28/94	5,684,907	11/04/97	Aerogel-Clad Optical Fiber
9385	A	Richard Pekala James Kaschmitter Steven Mayer	08/393588	02/21/95	5,623,977	05/06/97	Composite Carbon Foam Electrode
9385	B	Richard Pekala James Kaschmitter Steven Mayer	08/760852	12/02/96	5,898,564	04/27/99	Capacitor with a Composite Carbon Foam Electrode
9385	C	Richard Pekala James Kaschmitter Steven Mayer	09/246882	02/08/99	6,332,990	12/25/01	Composite Carbon Foam Electrode
9388	A	Richard Pekala	08/307219	09/16/94	5,476,878	12/19/95	Organic Aerogels from the Sol-Gel Polymerization of Phenolic-Furfural Mixtures
9388	B	Richard Pekala	08/429276	04/25/95	5,556,892	09/17/96	Organic Aerogels from the Sol-Gel Polymerization of Phenolic-Furfural Mixtures
9388	C	Richard Pekala	08/659377	06/06/96	5,744,510	04/28/98	Organic Carbon Aerogels from the Sol-Gel Polymerization of Phenolic-Furfural Mixtures
9471	A	Paul Coronado Lawrence W. Hrubesh John F. Poco	08/368823	01/05/95	5,686,031	11/11/97	Method For Rapidly Producing Microporous and Mesoporous Materials

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
		Robert W. Hopper					
9713	A	Joe Farmer Richard ARIE Vankonyn	09/072296	05/04/98	5,980,718	11/09/99	Means for Limiting and Ameliorating Electrode Shorting
9765	A	Lawrence W. Hrubesh Richard Pekala	08/610921	03/05/96	5,731,360	03/24/98	Compression Molding of Aerogel Microspheres
9833	A	Paul Coronado Lucy Hair Robert Sanner	08/767012	12/16/96	5,851,947	12/22/98	Incorporation of Noble Metals into Aerogels
9859	A	Paul Coronado John F. Poco	09/017035	02/02/98	5,973,015	10/26/99	Flexible Aerogel Composite for Mechanical Stability and Process of Fabrication
9859	B	Paul Coronado John F. Poco	09/379486	08/23/99	6,087,407	07/11/00	Flexible Aerogel Composite for Mechanical Stability And Process of Fabrication
9892	A	Lawrence W. Hrubesh John F. Poco	09/028040	02/23/98	6,168,737	01/02/01	Method of Casting Patterned Dielectric Structures
9904	A	Lawrence W. Hrubesh John F. Poco	09/039450	03/16/98	6,158,244	12/12/00	A Method of Producing Optical Quality Glass Having a Selected Refractive Index
10059	A	Paul Coronado Lawrence W. Hrubesh John F. Poco	09/182408	10/29/98	6,005,012	12/21/99	Method for Producing Hydrophobic Aerogels

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
10127	A	Lawrence W. Hrubesh Thomas Tillotson Randall L. Simpson Rosalind W. Swansiger Glenn Fox Ronald Lee	08/926357	09/09/97	6,666,935	12/23/03	Sol-Gel Manufactured Energetic Materials
10127	B	Lawrence W. Hrubesh Thomas Tillotson Randall L. Simpson Rosalind W. Swansiger Glenn Fox Ronald Lee	09/481043	01/11/00	Notice of Appeal Filed 9/2/08; Office Action: Filed Supplemental Appeal Brief; 3/17/09 Examiners Answer to Appeal Brief		Sol-Gel Manufactured Energetic Materials
10127	C	Lawrence W. Hrubesh Thomas Tillotson Randall L. Simpson Rosalind W. Swansiger Glenn Fox Ronald Lee	10/697477	10/29/03	6,893,518	05/17/05	Sol-Gel Manufactured Energetic Materials
10180	A	Thomas Tillotson Glenn Fox	10/393492	03/18/03	6,924,322	08/02/05	Thio-, Amine-, Nitro-, and Macrocyclic Containing Organic Aerogels and Xerogels
10192	A	Joe Farmer Laura Murguia Tri D. Tran	09/289876	04/12/99	6,309,532	10/30/01	Method and Apparatus for Capacitive Deionization and Electrochemical Purification and Regeneration of Electrodes

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
10220	A	Paul Coronado	10/253142	09/23/02	6,998,102	02/14/06	Rapid Process for Producing Transparent, Monolithic Porous Glass
10269	A	Paul Coronado	09/182409	10/29/98	5,958,363	09/28/99	Method for Making Monolithic Metal Oxide Aerogels
10287	A	Lawrence W. Hrubesh John F. Poco	09/970251	09/27/01	6,620,458	09/16/03	Method to Produce Alumina Aerogels Having Porosities Greater than 80%
10413	A	Lawrence W. Hrubesh	10/050437	01/15/02			Lightweight, High Strength Carbon Aerogel Composites and Method of Fabrication
10575	C	Alexander E. Gash Lawrence W. Hrubesh Thomas Tillotson Randall L. Simpson	09/981076	10/16/01	6,986,818	01/17/06	Method for Producing Nanostructured Metal-Oxides
10575	D	Lawrence W. Hrubesh Thomas Tillotson Randall L. Simpson	10/422488	04/24/03	6,986,819	01/17/06	Metal-Oxide Energetic Materials and Synthesis Thereof
10624	A	Paul Coronado Lawrence W. Hrubesh John F. Poco	10/002513	10/25/01	6,723,378	04/20/04	Fibers and Fabrics with Insulating, Water-Proofing, and Flame-Resistant Properties
10624	B	Paul Coronado Lawrence W. Hrubesh John F. Poco	10/746964	12/24/03	4/13/09 Examiners Answer - Reply Brief Filed		Fibers and Fabrics with Insulating, Water-Proofing, and Flame-Resistant Properties
10663	A	Paul Coronado	09/957854	09/21/01	6,709,600	03/23/04	Method for Removing

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
		Lawrence W. Hrubesh					Organic Liquids from Aqueous Solutions and Mixtures
10751	A	Paul Coronado Lawrence W. Hrusbesh John F. Poco	09/957853	09/21/01			Super-Hydrophobic Fluorine-Containing Aerogels
10751	B	Paul Coronado Lawrence W. Hrusbesh John F. Poco	10/794847	03/04/04	7,211,605	05/01/07	Super-Hydrophobic Fluorine-Containing Aerogels
10767	A	Joe Satcher Lawrence W. Hrubesh Thomas Tillotson Randall L. Simpson	10/132803	04/24/02	7,211,607	05/01/07	Method for Producing High Surface Area Chromia Materials for Catalysis
10781	A	Alexander E. Gash Joe Satcher Randall Simpson	10/186468	06/28/02	6,712,917	03/30/04	Inorganic Metal Oxide/Organic Polymer Nanocomposites and Method Thereof
10781	B	Alexander E. Gash Joe Satcher Randall Simpson	10/626098	07/23/03	6,818,081	11/16/04	Inorganic Metal Oxide/Organic Polymer Nanocomposites and Method Thereof
10788	A	Lawrence W. Hrubesh Raymond Brusasco Michael D. Feit Bernie Penetrante Alan Burnham Lloyd Hackel Mark R. Kozlowski Paul J. Wegne	09/948444	09/07/01	6,518,539	02/11/03	Method for Producing Damage Resistant Optics
10794	A	Thomas Tillotson Armando Alcaraz	10/163720	06/05/02	6,749,826	06/15/04	Carbon Nanotube Coatings as Chemical

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
		Brian D. Anderson					Absorbers
10837	A	Alexander E. Gash Joe Satcher Randall Simpson	11/165734	09/30/02	9/25/09 Examiner's Answer; 4/15/09 Non-Compliant Appeal Brief;		Preparation of Porous Pyrophoric Iron Using Sol-Gel Methods
10849	A	Theodore Baumann Alexander E. Gash Joe Satcher	10/132893	04/24/02	6,806,299	10/19/04	Preparation of Hydrophobic Organic Aerogels
10849	B	Theodore Baumann Alexander E. Gash Joe Satcher	10/927679	08/26/04	7,291,653	11/06/07	Preparation of Hydrophobic Organic Aerogels
10897	A	Theodore Baumann Joe Satcher	10/132783	04/24/02	6,613,809	09/02/03	Metal-Doped Organic Gels and Method Thereof
10897	B	Theodore Baumann Joe Satcher	10/457131	06/09/03	7,285,575	10/23/07	Metal-Doped Organic Gels and Method Thereof
10903	A	Paul Coronado Sabre Coleman John Reynolds	10/285242	10/30/02	6,806,227	10/19/04	Solid Materials for Removing Metals and Fabrication Method
10937	A	Paul Coronado Joe Satcher	11/335297	01/18/06			High Strength Air-Dried Aerogels
10963	A	Alexander E. Gash Joe Satcher Richard Landingham Randall Simpson Robert Reibold	10/447119	05/28/03	7,087,544	08/08/06	Nano-Ceramics and Method Thereof

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
11034	A	Alexander E. Gash Joe Satcher Randall Simpson Troy Barbee, Jr.	10/261879	09/30/02	5/5/09 12/11/08 Attorney elected not to respond to Examiner's Answer; 2/28/08 Appeal Brief;		Nano-Laminate-Based Ignitors
11187	A	Paul Coronado Theodore Baumann Joe Satcher Richard Landingham	11/479796	06/30/06	7/29/09 Office Action; 10/24/06 Confirmatory License		Forming Foam Structures with Carbon Foam Substrates
11234	A	Thomas Tillotson Kyle Fiet Alan Jankowski Nerine Cherepy	10/913573	08/05/04	3/30/09 Examiners Answer; Reply Brief Filed		Carbon Aerogel and Xerogel Fuels for Fuel Cells and Batteries
11258	A	Alexander E. Gash Joe Satcher David Sopchak Jeffrey Morse Ravindra Upadhye John Reynold	11/119047	04/28/05	11/07/08 Final Office Action: RCE filed with a 1 month Extension of Time; 9/28/05 Confirmatory License		Catalyst for Microelectromechanical Systems Microreactors [^]
11267	A	Lawrence W. Hrubesh Thomas Tillotson John F. Cooper	10/810477	03/26/04	7,410,718	08/12/08	Aerogel and Xerogel Composites for Use as Carbon Anodes
11267	B	Lawrence W. Hrubesh Thomas Tillotson John F. Cooper	12/118571	05/09/08			Aerogels and Xerogels Composites for use as Carbon Anodes
11286	A	Paul Coronado Robert Sanner John Reynolds Victoria Dias	10/728568	12/04/03	7,393,810	07/01/08	Solid Materials for Removing Arsenic and Method Thereof

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
		Sabre Coleman					
11286	B	Paul Coronado Robert Sanner John Reynolds Victoria Dias Sabre Coleman	12/134700	06/06/08			Solid Materials for Removing Arsenic and Method Thereof
11287	A	Paul Coronado Sabre Coleman John Reynolds	10/794853	03/04/04	7,148,180	12/12/06	Composites for Removing Metals and Volatile Organic Compounds and Method Thereof
11561	A	Alexander E. Gash Joseph Tringe Troy Barbee, Jr.	11/484543	06/28/06	6/10/09 Notice of Allowance; 10/24/06 Confirmatory License		Electrical Initiation of an Energetic Nanolaminate Film
11634	A	Alexander E. Gash Troy Barbee, Jr.	11/804454	05/18/07	7/10/07 Confirmatory License		Energetic Composite and System with Enhanced Mechanical Sensitivity to Initiation of Self-Sustained Reaction
11698	A	Thomas Tillotson Nerine Cherepy Joshua Kuntz Stephen Payne	11/805275	05/21/07			Fabrication of Transparent Ceramics Using Nanoparticles
11706	A	Alexander E. Gash Joe Satcher Randall Simpson Richard Landingham Robert Reibold	11/477331	06/28/06			Nano-Ceramics and Method Thereof

Docket Number	10	Inventor	Application Number	Filing Date	Patent Number	Issue Date	Patent Title
11829	A	Alexander E. Gash Joe Satcher Randall Simpson Richard Landingham Joshua Kuntz	12/580185	10/15/09			Fabrication and Processing of Energetic Composite Materials
11850	A	Alexander E. Gash Thomas Yong-Jin han Donald Sirbuly	12/392025	02/24/09			Organized Energetic Composites Based on Micro and Nanostructures and Methods Thereof
11907	1	Theodore Baumann Alexander E. Gash Joe Satcher Randall Simpson Marcus Worsley	12/329437	12/05/08			Pyrophoric Metal-Carbon Foam Composites

Appendix 4: Additionality of ARPA-E Funding

This seedling proposal requests \$500K over two years with a 20% in-kind match by the industrial partner, Ocellus for execution of tasks 1 through 8, the initial demonstration of the concept. These funds will be required to demonstrate the feasibility of using ultra-high surface area carbon aerogels, or other alternatives that may evolve during the research, as adsorption media in a solar-powered aerogel-based adsorptive refrigeration cycle. Without crucial funding from ARPA-E, the suitability of using these novel and proprietary materials, originally developed by the Department of Energy, will probably not be determined.

Appendix 5: Tasks, Deliverables & Milestones Details

	FY1				FY2			
Tasks, Milestones & Deliverables	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1 – Initial Synthesis of Ultrahigh Surface Carbon Aerogel								
Deliverable 1.1: Procurement of Materials and Chemicals								
Deliverable 1.2: Synthesis of 1st 5-kg Batch of UHS-CA with BET Surface Area > 3000 m ² /g								
Task Duration: 6 Months								
Task 2 – Determination of Adsorption Isotherms								
Deliverable 2.1: Design & Construction of Apparatus for Isotherm Determination								
Deliverable 2.2: Adsorption Isotherms for Halogenated Refrigerants & Conventional AC								
Deliverable 2.3: Adsorption Isotherms for Halogenated Refrigerants & UHS-CA								
Deliverable 2.4: Adsorption Isotherms for Non-Halogenated Refrigerants & Conventional AC								
Deliverable 2.5: Adsorption Isotherms for Halogenated Refrigerants & UHS-CA								
Duration: 9 Months								
Task 3 – Production Synthesis UHS-CA								
Deliverable 3.1: Procurement of Additional Materials and Chemicals								
Deliverable 3.2: Synthesis of 2nd 100-kg Batch of UHS-CA with BET Surface Area > 3000 m ² /g								
Duration: 6 Months								
Task 4 – Quality Assurance & Quality Control of UHS-CA Production								
Deliverable 4.1: ESEM, EDAX & TEM of Representative Samples from 1st 5-kg Batch of UHS-CA								

	FY1				FY2			
Tasks, Milestones & Deliverables	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Deliverable 4.2: Determination of Density and BET Surface Area for 1st 5-kg Batch of UHS-CA								
Deliverable 4.3: ESEM, EDAX & TEM of Representative Samples from 2nd 100-kg Batch of UHS-CA								
Deliverable 4.4: Determination of Density and BET Surface Area for 2nd 100-kg Batch of UHS-CA								
Deliverable 4.5: Adsorption Isotherms for Refrigerant Candidate A on 2nd 100-kg Batch of UHS-CA								
Deliverable 4.6: Adsorption Isotherms for Refrigerant Candidate B on 2nd 100-kg Batch of UHS-CA								
Duration: 12 Months								
Task 5 – Computational Analysis & Design of System								
Deliverable 5.1: Conceptual Design of Single-Bed Prototype								
Deliverable 5.2: Preliminary Spreadsheet Model of Single-Bed System								
Deliverable 5.3: Comprehensive Computational Model for Transient Operation								
Deliverable 5.4: Initial Calibration of Model Parameters with Adsorption Isotherm Data								
Deliverable 5.5: Thermal Analysis of Single-Bed Prototype								
Duration: 6 Months								
Task 6 – Engineering Design of Single-Bed System & Components								
Deliverable 6.1: Engineering Drawings for Construction of Single-Bed Prototype								
Deliverable 6.2: Engineering Drawings of Components for Single-Bed Prototype								
Deliverable 6.3: Procure Commercially Available Components for Single-Bed Prototype								
Duration: 3 Months								

	FY1				FY2			
Tasks, Milestones & Deliverables	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 7 – Component Fabrication, Charging Adsorption Bed, Assembly & Installation								
Deliverable 7.1: Fabricated Components for Single-Bed Prototype								
Deliverable 7.2: Procured Components for Single-Bed Prototype								
Deliverable 7.3: Procured Components for Single-Bed Prototype								
Deliverable 7.4: Charging of Adsorption Bed for Single-Bed Prototype Assembly								
Deliverable 7.5: Fully Assembled of Single-Bed Prototype								
Deliverable 7.6: Installation of Assembled Single-Bed Prototype on HVAC Laboratory								
Duration: 6 Months								
Task 8 – Performance Testing and Demonstration								
Deliverable 8.1: Successful Performance Test of Single-Bed Prototype with Electrical Heater								
Deliverable 8.2: Successful Performance Test of Single-Bed Prototype with Solar Heating								
Deliverable 8.3: Report Documenting Data from Performance Testing of Single-Bed Prototype								
Duration: 6 Months								
Task 9 – Calibrated & Validated Computational Model for System Design								
Deliverable 9.1: Successful Performance Test of Single-Bed Prototype with Electrical Heater								
Deliverable 9.2: Calibration of Model Parameters with Data from Single-Bed Prototype Testing								
Deliverable 9.3: Independent Experiment for Model Validation								
Duration: 3 Months								

	FY1				FY2			
Tasks, Milestones & Deliverables	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 10 – Design & Optimization of Two-Bed Temperature-Swing Prototype								
Deliverable 10.1: Conceptual Design of Two-Bed Temperature-Swing System								
Deliverable 10.2: Reconfiguration of Computational Model for Simulation of Two-Bed System								
Deliverable 10.3: Optimization of Two-Bed Temperature-Swing System								
Deliverable 10.4: Engineering Drawings for Two-Bed Temperature-Swing System								
Deliverable 10.5: Physical Reconfiguration of System as Two-Bed Temperature Swing System								
Duration: 6 Months								
Task 11 – Performance Testing & Demonstration of Two-Bed Temperature-Swing Prototype								
Deliverable 11.1: Testing of Two-Bed Temperature-Swing Prototype with Electrical Heaters								
Deliverable 11.2: Testing of Two-Bed Temperature-Swing Prototype with Solar Heating								
Deliverable 11.3: Report on Testing of Two-Bed Temperature-Swing Prototype								
Duration: 6 Months								
Task 12 – High Performance Thermal Insulation Enhancement								
Deliverable 12.1: Synthesis of Silica Aerogel for Enhanced Thermal Insulation								
Deliverable 12.2: Retrofit of Two-Bed Temperature-Swing Prototype with Aerogel Insulation								
Deliverable 12.3: Performance Test of System with Enhanced Insulation								
Duration: 6 Months								
Task 13 – Technology Transfer & Commercialization								

	FY1				FY2			
Tasks, Milestones & Deliverables	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Deliverable 12.1: Comprehensive Records of Invention for Single- and Multi-Bed Systems								
Deliverable 12.2: Comprehensive Patent Applications for Single- and Multi-Bed Systems								
Deliverable 12.3: Copyrights for Pertinent Branding and Trademarks								
Deliverable 12.4: Formal Agreements for Non-LLNL Site Demonstrations								
Deliverable 12.5: One Successful Non-LLNL Site Demonstration								
Deliverable 12.6: Industry Days at LLNL in Collaboration with DOE EERE Program Manager								
Deliverable 12.7: Field of Use Licenses for Aerogel-Based Cooling Systems								
Duration: 36 Months								